IRI: What novel interfaces will HPC expose for cross-facility workflows?

Why are we here today?

- HPC has seen a rise in non-traditional use cases:
  - Complex cross- facility workflows
  - Data/Analysis-centric users
  - Machine-to-machine workflows
- Evidence in multiple projects
  - Superfacility/SENSE/Intersect/ACE (OLCF)
  - Blueprints of DOE's Integrated Research Infrastructure (IRI)
- New class(es) of users and use cases
  - Machine/Service/Collab accounts
  - Data/Analysis-centric users
  - HPC integration in data/ML workflows from other facilities
- To service these use cases we need to step out of our "shell" and provide alternative interfaces
  - APIs
  - Workflow orchestrators
  - UIs (Jupyter etc)
- Landscape of interfaces is rather fragmented today
  - DOE's IRI seeks to harmonize this at least for ASCR facilities
  - Opportunity to create interfaces that facilitate cross-facility workflows

Think!

- What would you like alternative interfaces to look like?
- What are the difficulties with your current cross-facility workflow?

Agenda

12:15-12:20 Welcome and opening remarks
Bjoern Enders, National Energy Research Scientific Computing Center (NERSC)

12:20-12:25 Introduction to the IRI interfaces subcommittee and charter
John MacAuley, Energy Sciences Network (ESnet)

12:25-12:50 Lightning Talks

Superfacility API and Jupyter
Bjoern Enders, National Energy Research Scientific Computing Center (NERSC)

Cross-Facility Science Workflows Automation and Orchestration
Xi Yang, Energy Sciences Network (ESnet)

Services for integrating Data Portals
Ryan Prout, Oak Ridge Leadership Computing Facility (OLCF)

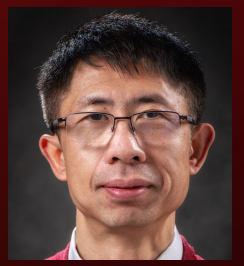
Globus Platform Interfaces for Automating Science
Kyle Chard, Argonne National Lab (ANL)

FirecREST: an Open-Source API for HPC
Juan Pablo Dorsch, CSCS

12:50 -1:15 Panel discussion and Open Q&A

Bjoern Enders
NERSC/LBL

John MacAuley
ESnet



Xi Yang
ESnet

Ryan Prout
OLCF

Ilya Baldin
JLAB

Juan Pablo Dorsch
CSCS

Kyle Chard
ANL

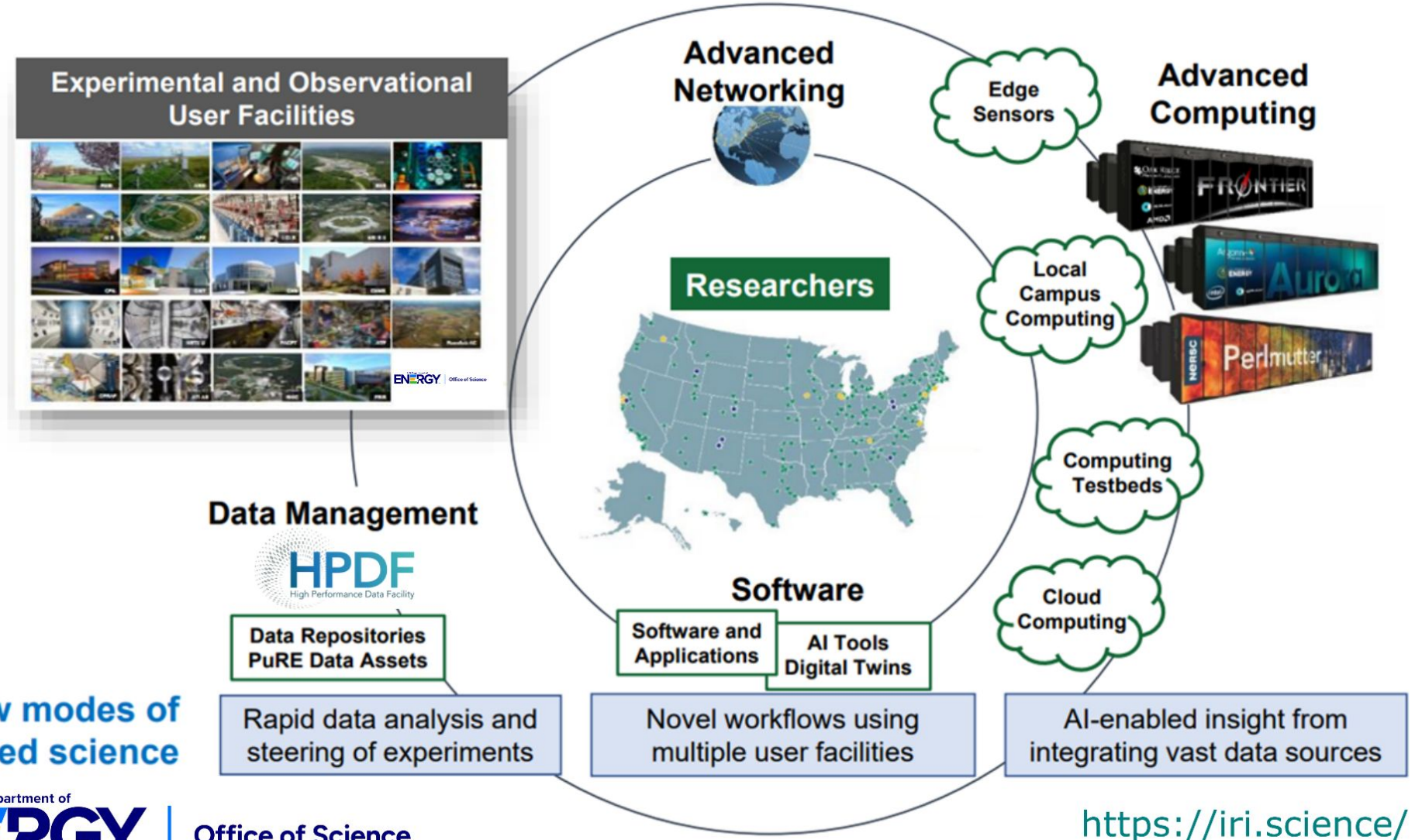
Please hold your questions until the Q&A

IRI technical subcommittee

John MacAuley
Energy Sciences Network (ESnet)

DOE's Integrated Research Infrastructure (IRI) Vision

To empower researchers to meld DOE's world-class research tools, infrastructure, and user facilities seamlessly and securely in novel ways to radically accelerate discovery and innovation.



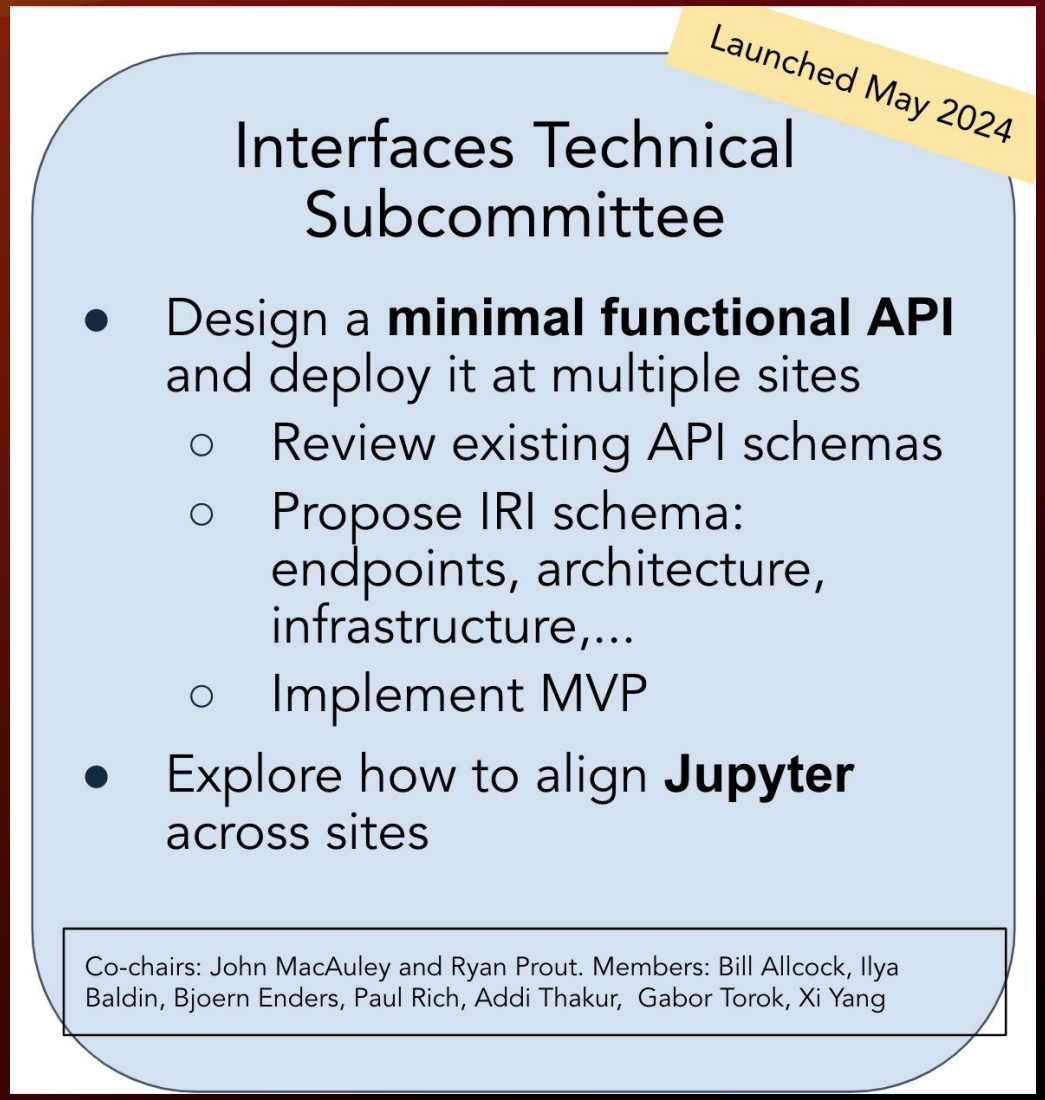
New modes of integrated science

U.S. Department of ENERGY | Office of Science

https://iri.science/

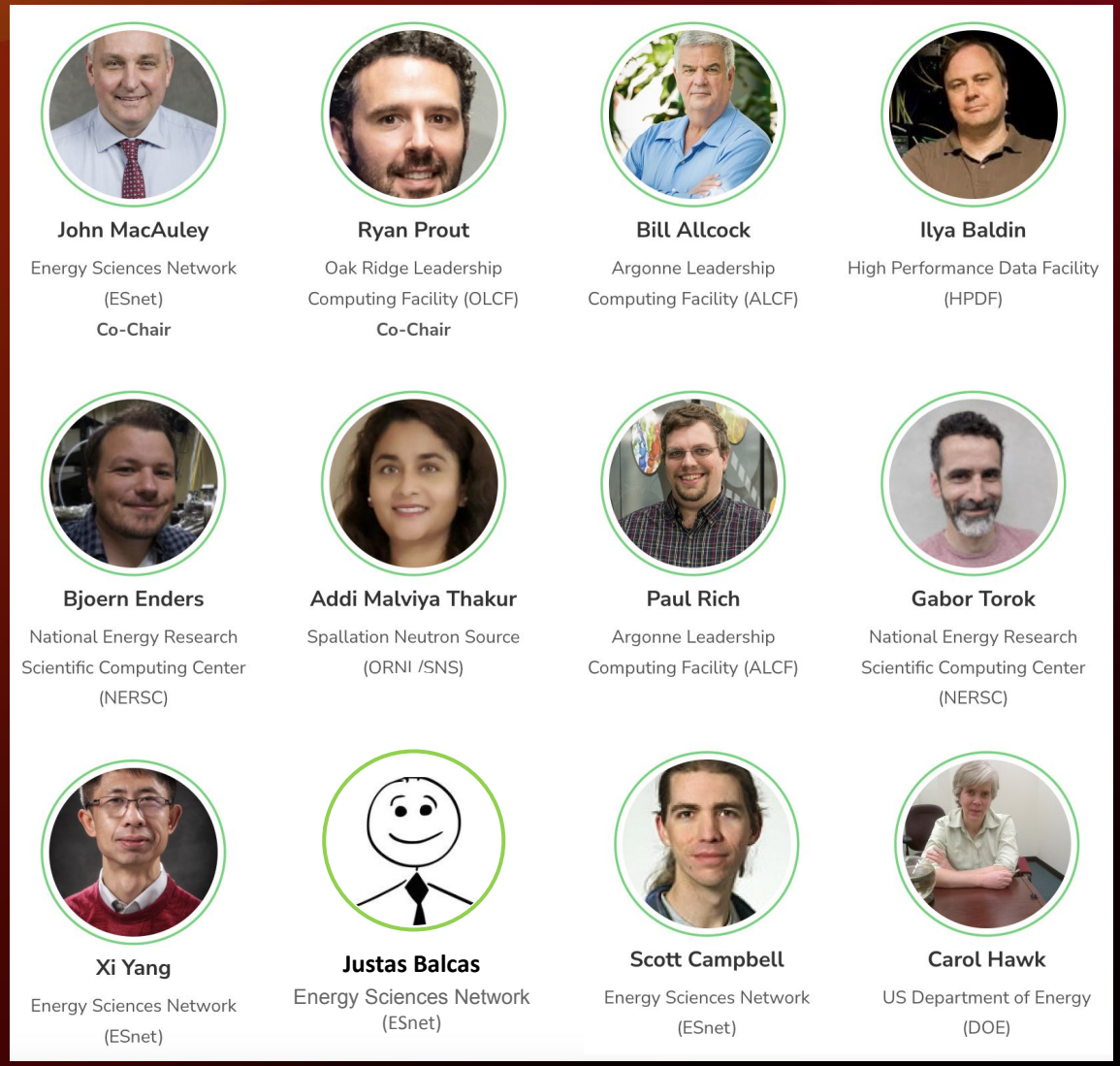
IRI Interfaces Charter

- Gather requirements, define use cases, and specify unified interfaces for the DOE ASCR Facilities.
- Tasked with enhancing the "user experience" for interaction and management of complex workflows across ASCR facilities
  - ➢ Goal is to facilitate a more cohesive and efficient research infrastructure.
- Consider applicable standards and build upon the work of other organizations where available to deliver a reference IRI interface implementation.



Status

- Team formation complete
  - But always looking for eager participants!
- Delivered
  - Subcommittee charter.
  - 2-year development roadmap.
- Developed a shared understanding
  - Different experiences, technologies, and terminologies.
- Actively defining a Facility Status API
  - Use case and requirements definition.
  - Modelling and protocol definition.
- Cross-pollinating subcommittees
  - TRUSTID, Outreach and Engagement.



Lightning Talk I

Superfacility API and Jupyter

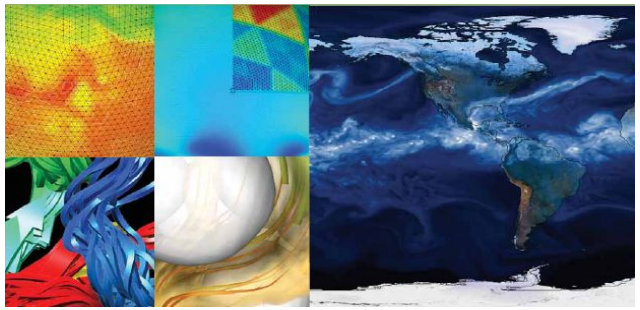
Bjoern Enders
NERSC

SC24
Atlanta, GA | hpc creates.

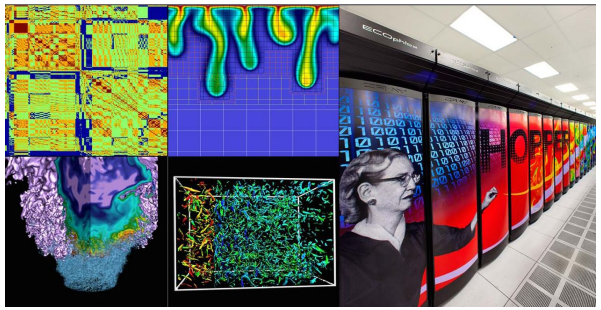
NERSC is the Production HPC & Data Facility for DOE Office of Science Research

U.S. DEPARTMENT OF ENERGY | Office of Science

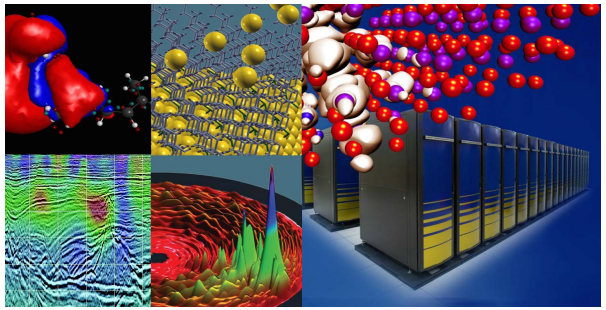
Largest funder of physical science research in U.S.



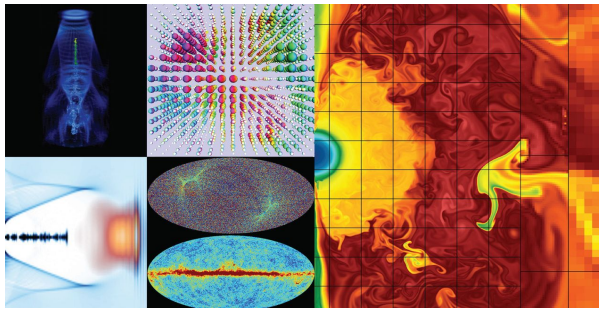
Biology, Energy, Environment



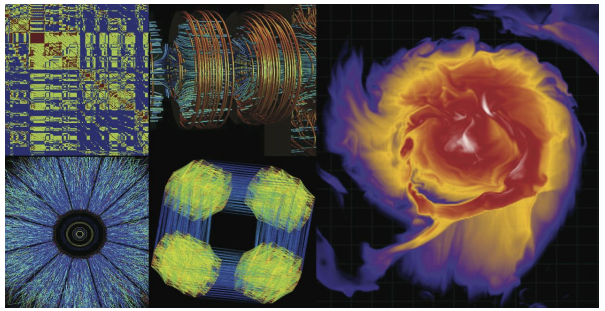
Computing



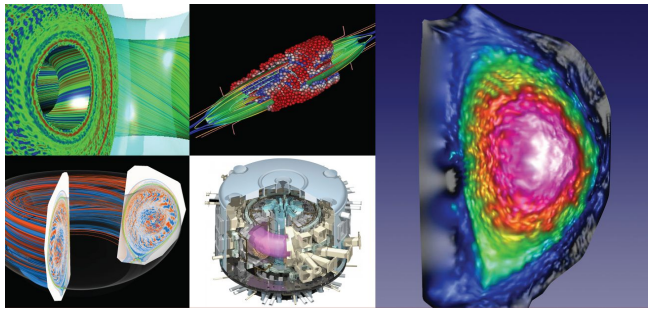
Materials, Chemistry, Geophysics



Particle Physics, Astrophysics



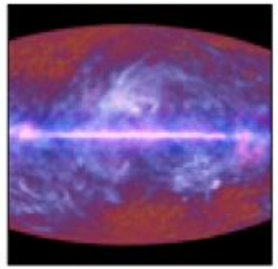
Nuclear Physics



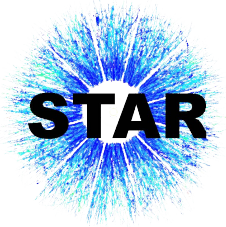
Fusion Energy, Plasma Physics

NERSC supports a large number of users and projects from DOE SC's experimental and observational facilities

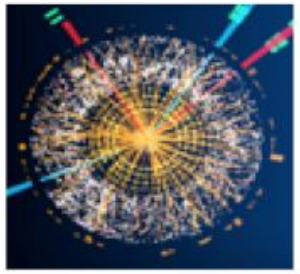
Palomar Transient Factory
Supernova



Planck Satellite
Cosmic Microwave Background
Radiation

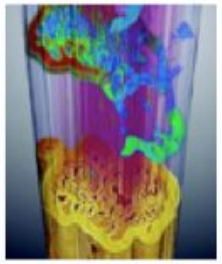


Star
Nuclear Physics



Atlas
Large Hadron Collide

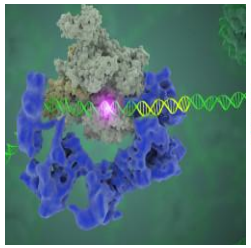
Dayabay
Neutrinos



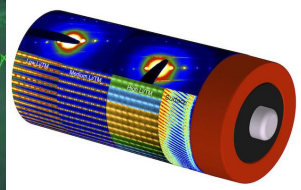
ALS
Light Source

LCLS
Light Source

Joint Genome Institute
Bioinformatics



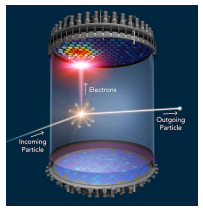
Cryo-EM



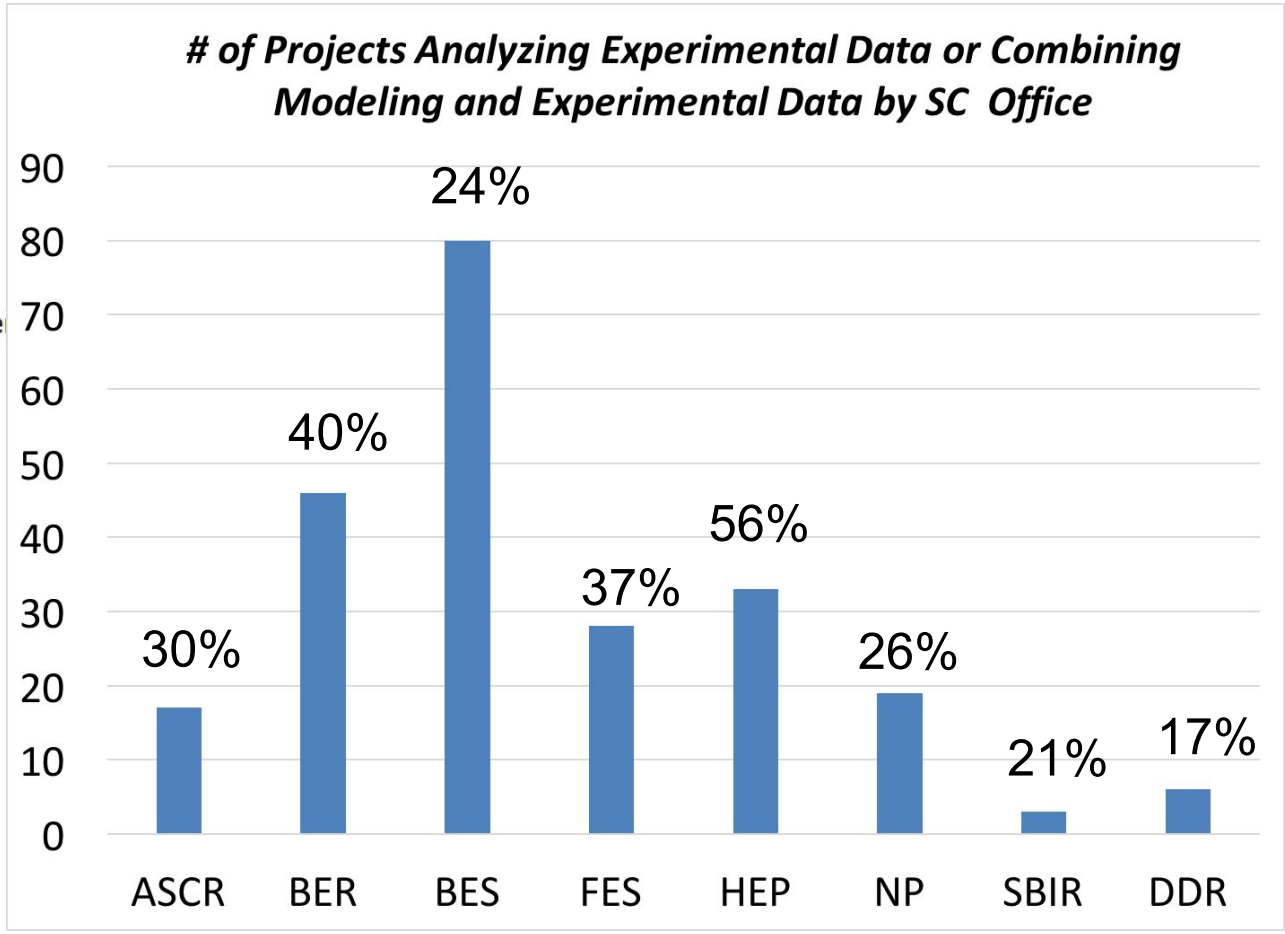
NCEM

DESI

LSST-DESC



LZ

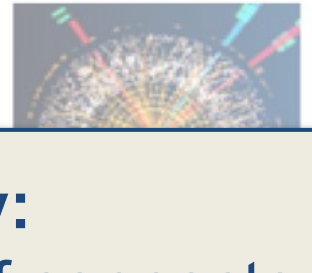


~35% (235) of NERSC projects self identified as confirming the primary role of the project is to 1) analyze experimental data or; 2) create tools for experimental data analysis or; 3) combine experimental data with simulations and modeling

NERSC supports a large number of users and projects from DOE SC's experimental and observational facilities

Palomar Transient Factory Supernova

Planck Satelli Cosmic Micro Background Radiation

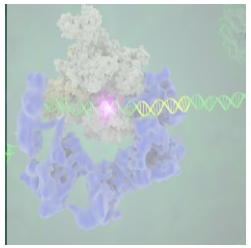


Dayabay Neutrinos

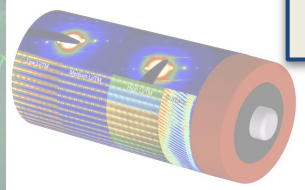
ALS Light Source

Superfacility:
Ecosystem of connected facilities, software and expertise to enable new modes of discovery

Superfacility API:
An API into NERSC to embed HPC into cross-facility workflows. It is also a general purpose API for all NERSC users and projects.



Cryo-EM



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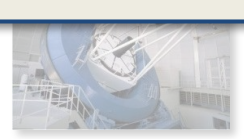

DESI

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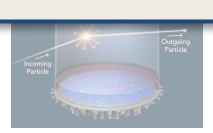

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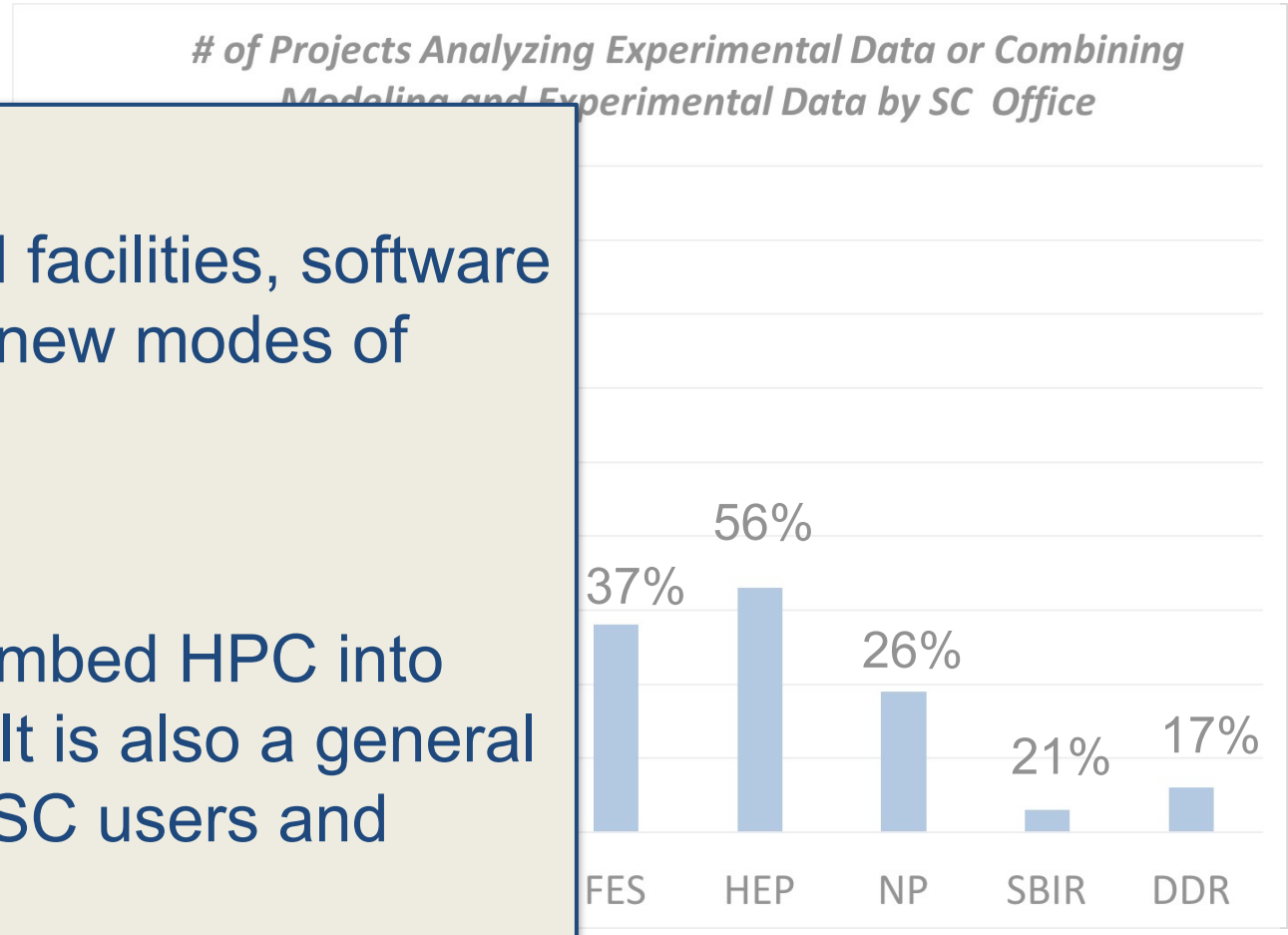

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Why an API?

- **Meets a critical need; automation is no longer optional**
  - Unattended operation; minimizing HITL
  - Track/submit large number of jobs
  - Interface with collaborations, workflows and machines
- **NERSC becomes "machine readable"**
  - Enables easier creation of UIs, portals, etc.
  - Allows integration with control/analysis software
    - " NERSC inside™ "
- **Less DIY: simpler, standardized tooling (Python, etc)**
  - Stable refactor target for established projects or easier on-ramp for new ones
  - Contribute to HPC interface standards for portability
  - Authentication and security models

Drivers:

- **Complex workflows**
- **Data-driven projects**
- **Real-time compute and streaming data from instruments**
- **Automation**

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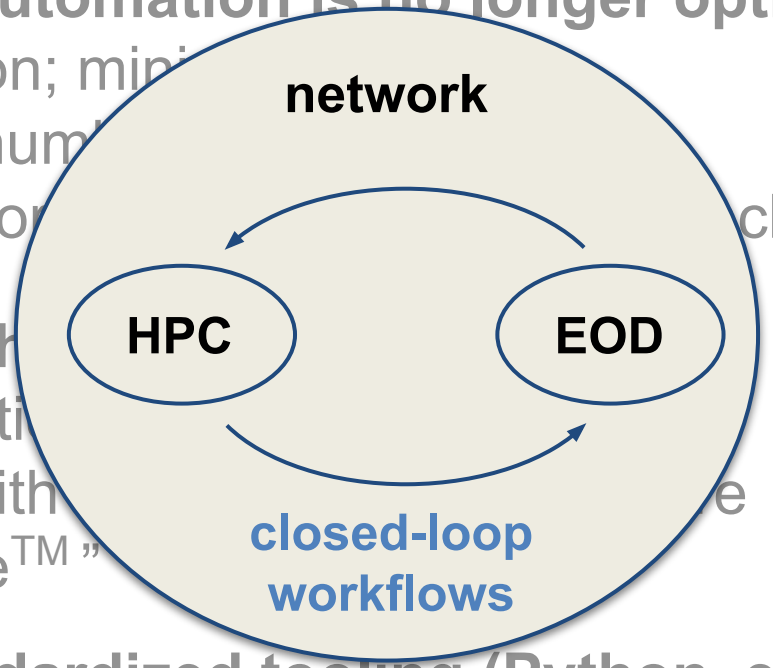


Drivers:

- **Complex workflows**
- **Data-driven projects**
- **Real-time compute and streaming data from instruments**
- **Automation**

What is the API good for?

Vision: all NERSC interactions are callable to facilitate seamless, automated "NERSC inside" workflows without a human in the loop.

Endpoints

- /status
- /account
- /compute
- /storage
- /tasks
- /utilities
- ../beta

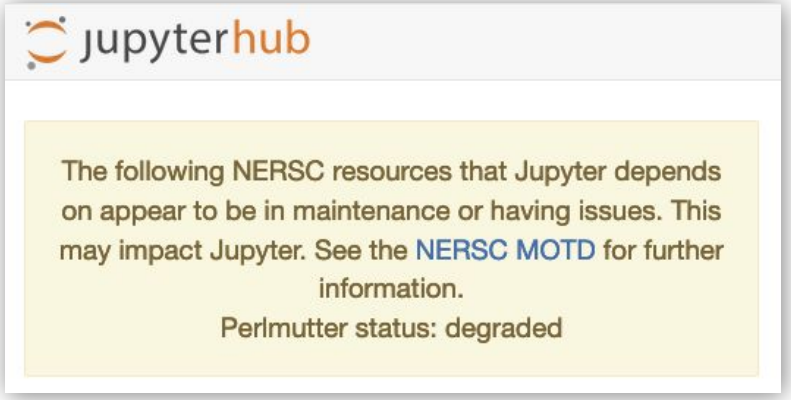
Example request

```
curl -X 'GET' \
  'https://api.nersc.gov/api/v1.2/status/perlmutter' \
  -H 'accept: application/json'
```

Result:

```
{
  "name": "perlmutter",
  "full_name": "Perlmutter",
  "description": "System is active",
  "system_type": "compute",
  "notes": [],
  "status": "active",
  "updated_at": "2023-03-02T18:00:00-08:00"
}
```

API is used both internally at NERSC and externally for our users



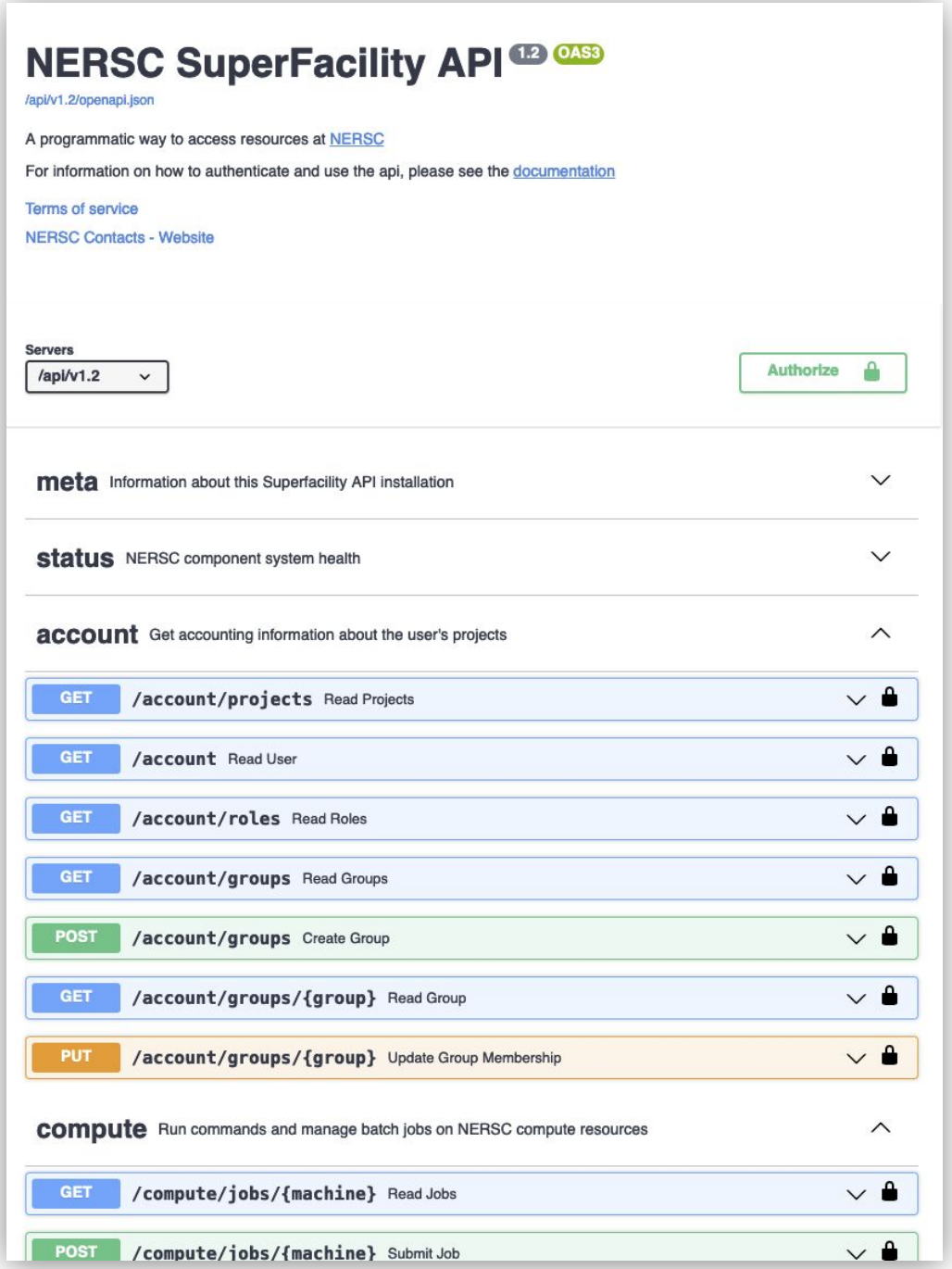
Interface documentation

https://api.nersc.gov/api/v1.2

- Interactive, up-to-date and self-documenting
- See endpoints, payloads, example code
- Works with any dev environment
- *Endpoints with significant work are asynchronous*
- End user docs and examples: https://docs.nersc.gov/services/sfapi/

Authorization

- Some endpoints are public and don't need an access token (no lock icon)
- For authorized endpoints (with lock icon), click the "Authorize" button at the top page and paste the access token



Projects using the SF API

Since release in 2022 (Feb 2023 numbers)

- 27 non-staff users made clients
- members of 40 different non-staff projects.

~ 12M logged requests from May 2022 - Feb 2023

= one request every 2 sec

Examples

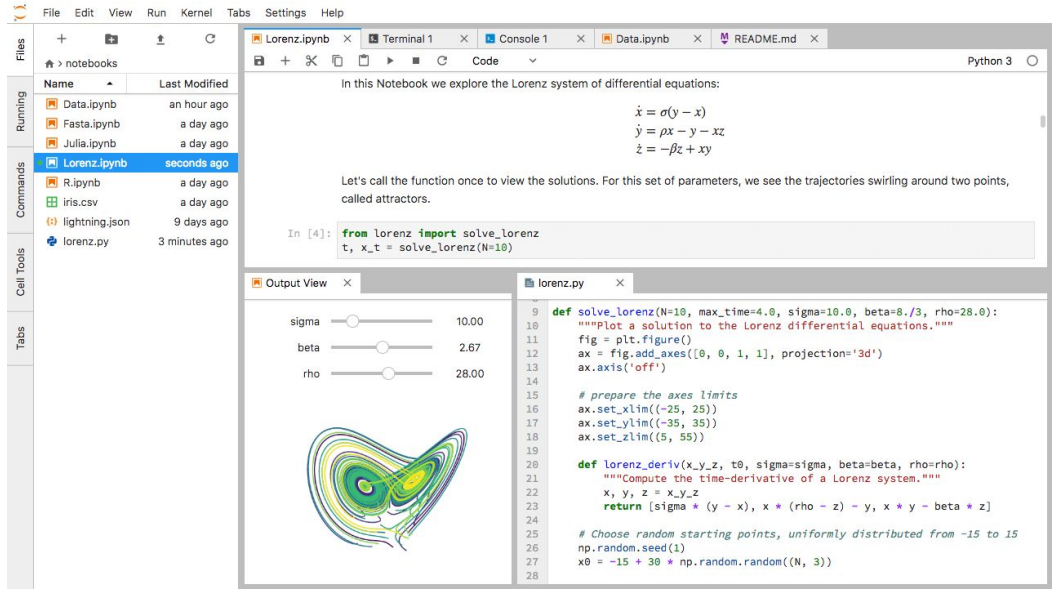
automated data processing for serial diffraction/scattering workflows

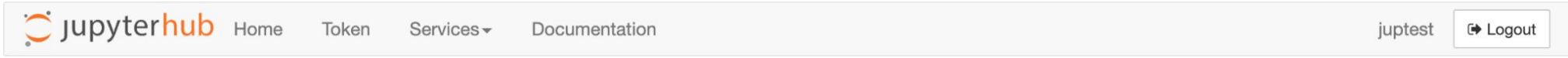
automated processing (HTC) of 4D STEM scan data with the Distiller app.

automated data processing between each of their plasma shots to reconstruct the shape and properties of the plasma.

Jupyter at NERSC

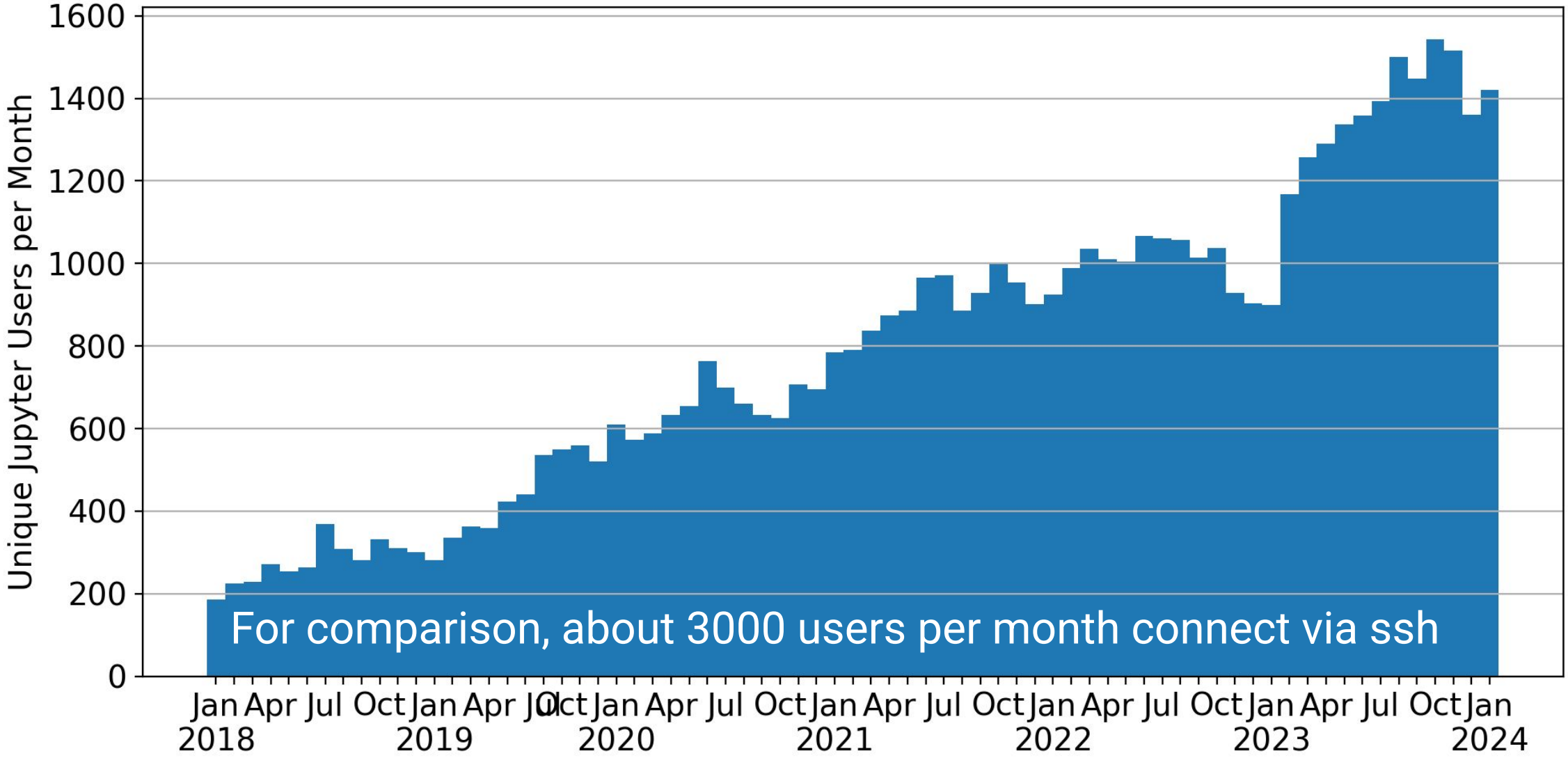
- Hosted at jupyter.nersc.gov
- Invaluable component of NERSC's data intensive science portfolio
  - Data cleaning and data transformation
  - Numerical simulation
  - Machine learning
  - Workflows and analytics frameworks
  - ….
- Configurable notebook servers
  - Shared, CPU/GPU, reservations
- Comes with NERSC's conda env
  - but run your own conda env,, container etc.





	Shared CPU Node	Exclusive CPU Node	Exclusive GPU Node	Configurable Job
Perlmutter	start	start	start	start
Resources	Use a node shared with other users' notebooks but outside the batch queues.	Use your own node within a job allocation using defaults.		Use multiple compute nodes with specialized settings.
Use Cases	Visualization and analytics that are not memory intensive and can run on just a few cores.	Visualization, analytics, machine learning that is compute or memory intensive but can be done on a single node.		Multi-node analytics jobs, jobs in reservations, custom project charging, and more.

Jupyter Usage at NERSC



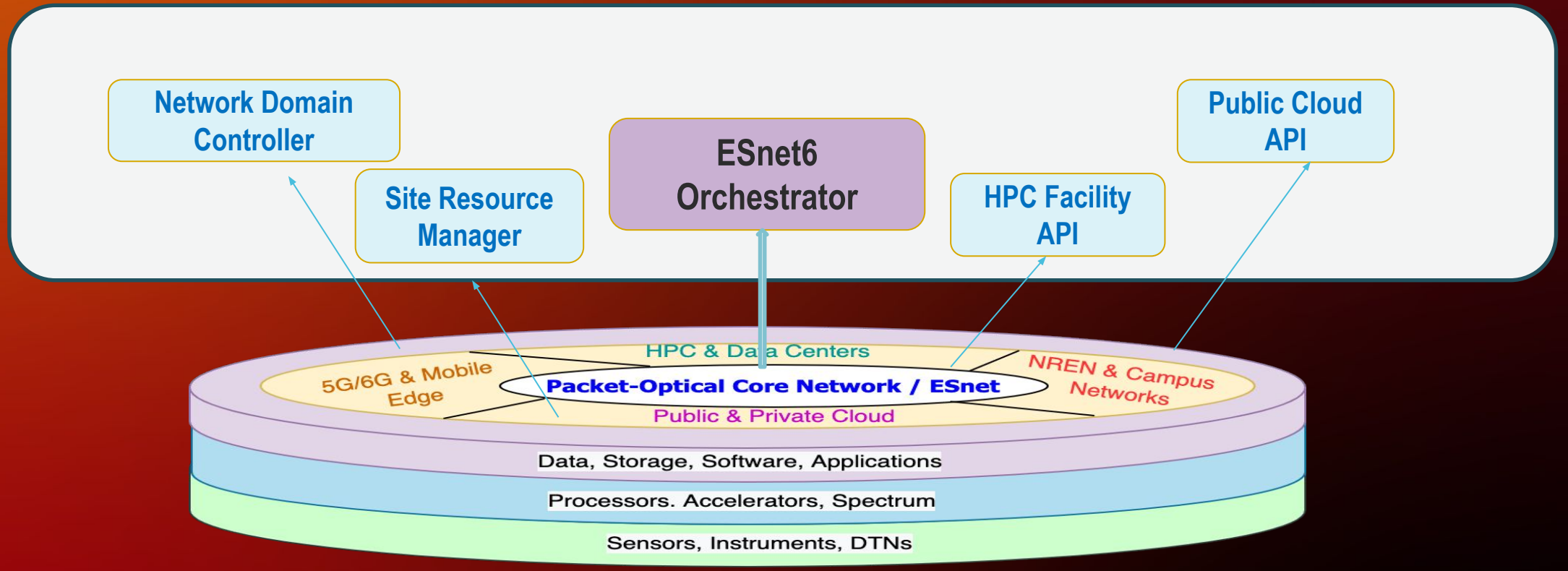
Lightning Talk II

Cross-Facility Science Workflows Automation and Orchestration

Xi Yang
Energy Sciences Network (ESnet)

SC24
Atlanta, GA | hpc creates.

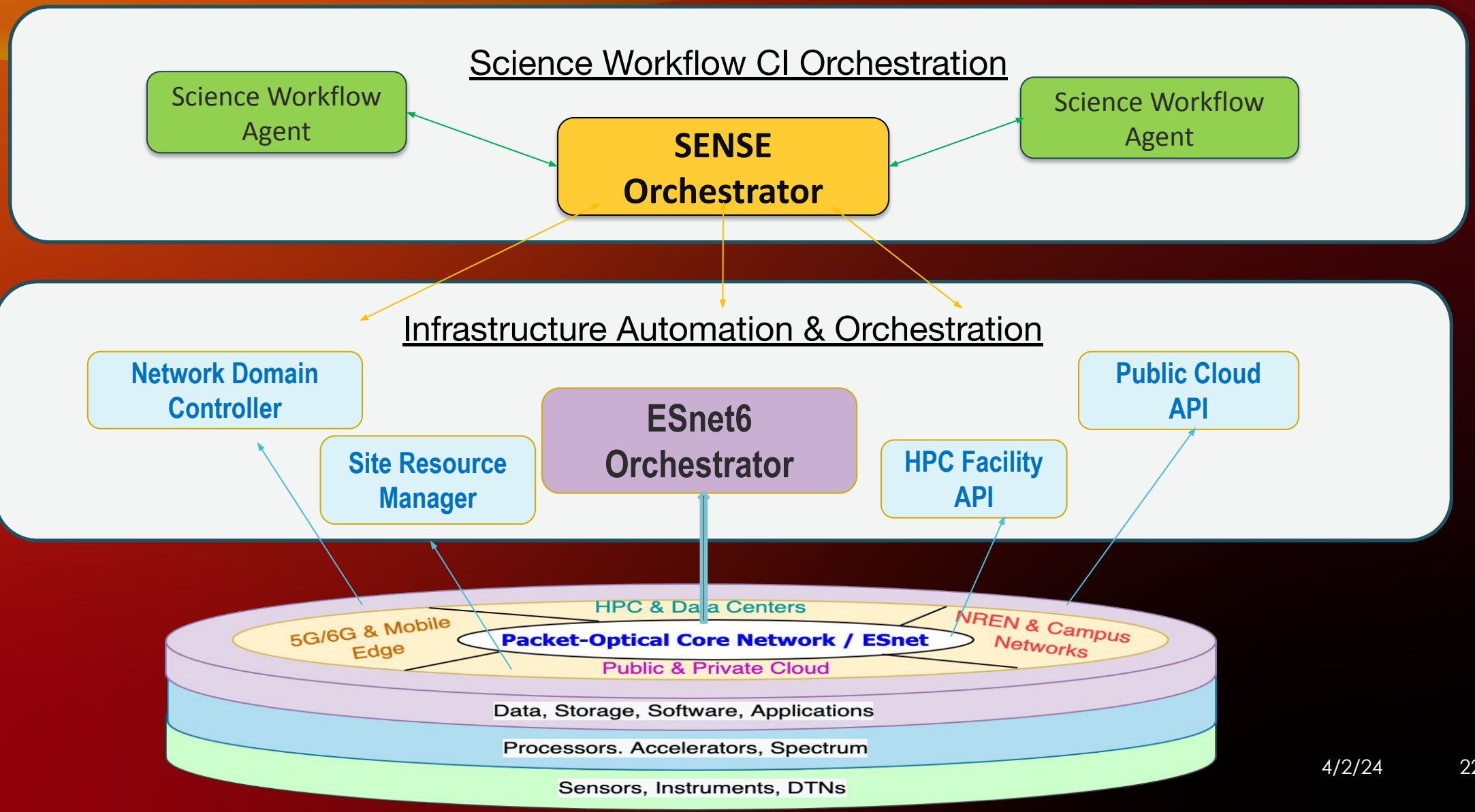
Facility Infrastructure Automation and Orchestration



Cross-Facility Fundamentals

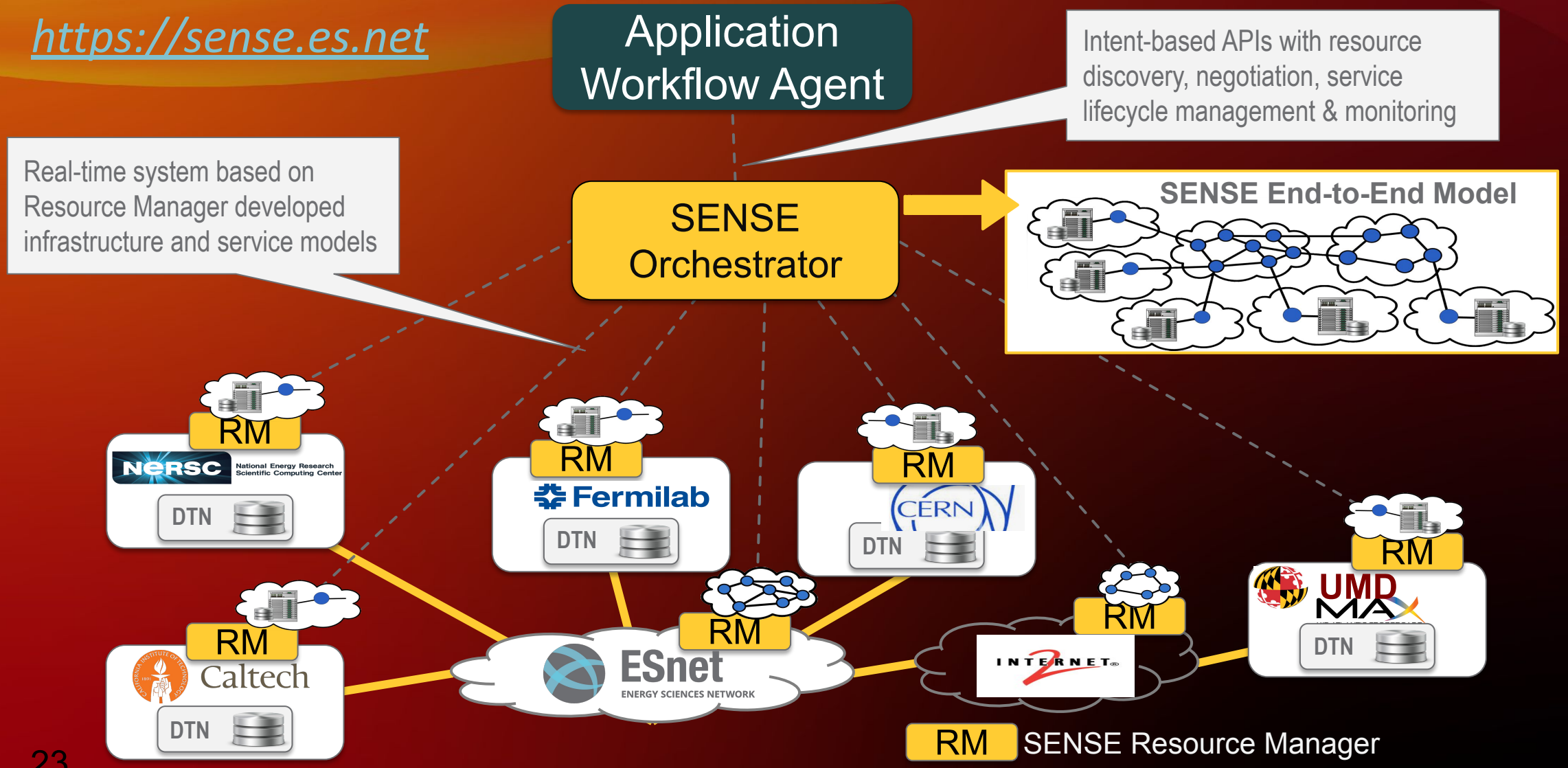
- **Connection**
  - Foundation level: L1 / L2 / L3
- **Identity**
  - Federated IDs to access native and external resources.
- **Facility API**
  - Facilities may use common APIs and common information models
  - Enforcement and maintenance of API interworking can be challenging
- **Workflow Tool**
  - Besides common API, workflow tools may understand multiple APIs, allocate resources on multiple facilities, and create connections between them.

Cross-Facility Science Workflows Automation and Orchestration



SENSE - An Example API-Based Cross-Facility Architecture

https://sense.es.net



SENSE Recommended Best Practices for Cross-Facility API

- “Functional” API is more important than “same” API
- Deterministic, negotiable and reservable services are the key
- Provides consistent resource model, service and policy definitions
- Offload orchestration intelligence to middleware
- Middleware normalizes your interface with the “plural” APIs
- Workflow agents Interact with middleware by iterating on what-if questions, agreements and feedbacks on behalf of user applications

Extrapolation – The Questions to Ask

- **API Structure**
  - What does a “Common API” means?
  - Is it a single specification, a set or a hierarchy of APIs?
  - Is north-south API interaction between workflow and facilities enough or we also need east-west facility interactions?
- **Information Model**
  - Can we build an ecosystem of universal ontologies and semantics?
  - Can we agree on a common resource modeling language and method?
  - What are the most important common functions?
- **Access Policy**
  - Can we normalize user identity and attributes across facility IdPs?
  - Can we represent / translate workflow policy to facility native policies?
  - Do we need a global clearinghouse? (enforcement)

Lightning Talk III

Services for integrating Data Portals

Ryan Prout
Oak Ridge Leadership Computing Facility (OLCF)

What is the OLCF?

The OLCF supports research in biology, chemistry, seismology, engineering, energy, and many other fields. **OLCF simulations have improved the safety and performance of nuclear power plants, turbomachinery, and aircraft; accelerated development of new drugs and advanced materials; and informed design of an international fusion reactor**. The simulations have explored hurricanes, biofuels, neurodegenerative diseases, and clean combustion for power and propulsion.

Multi-enclave HPC ecosystem

Defining different avenues of exploration *(an HPC Facility perspective)*

Facility-developed portals and workflow orchestration systems

- Objective is to enhance the local and unique facility ecosystem

Externally-developed data portals and workflow orchestration systems

- Objective is to extend the local facility ecosystem to an external system

Augment the HPC experience and large-scale simulation workflow, from running jobs to sharing data and insight with a larger community

Operational challenges of externally developed data portals and workflow orchestration systems *(an HPC Facility perspective)*

Policy and New Modes of Trust

Integration and access

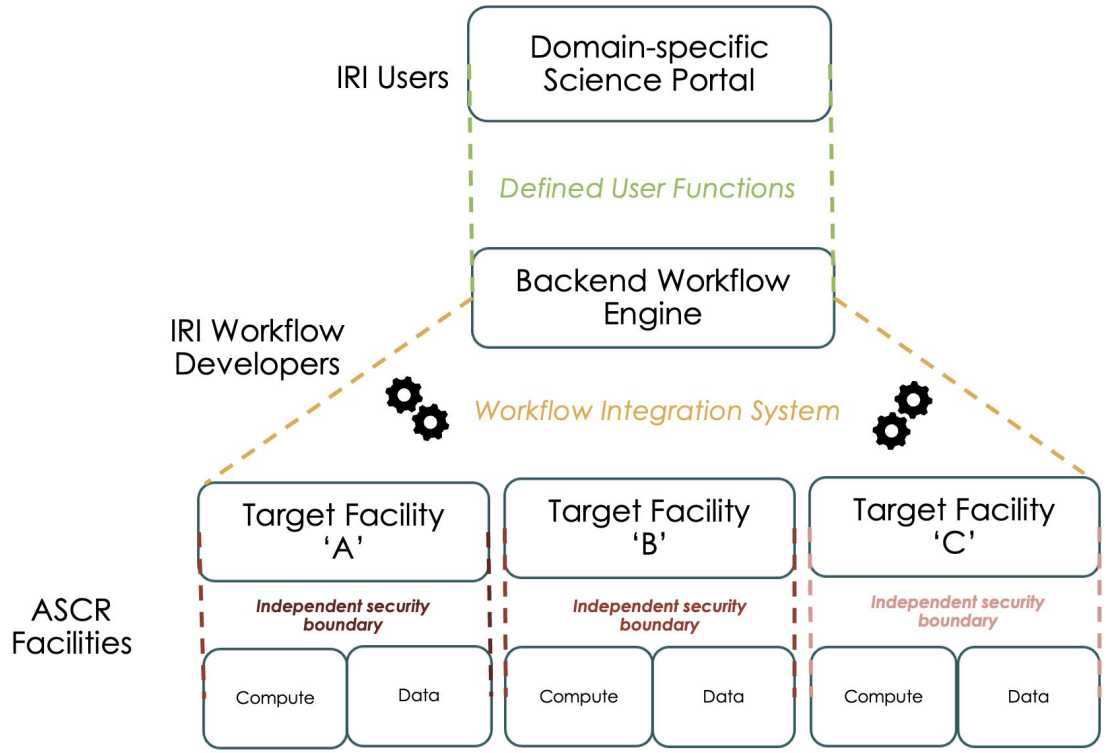
- Emphasis on software-to-software interaction (APIs and services instead of users and SSH sessions)
- Authentication and authorization
  - How do we trust external users and authorize them through third-party workflow systems?

Software Engineering

Extending access to protected facility resources

- Extend access to facility provided resources to the outside world in new and *secure* ways
- Meet policy requirements
- External developer experience and user experience

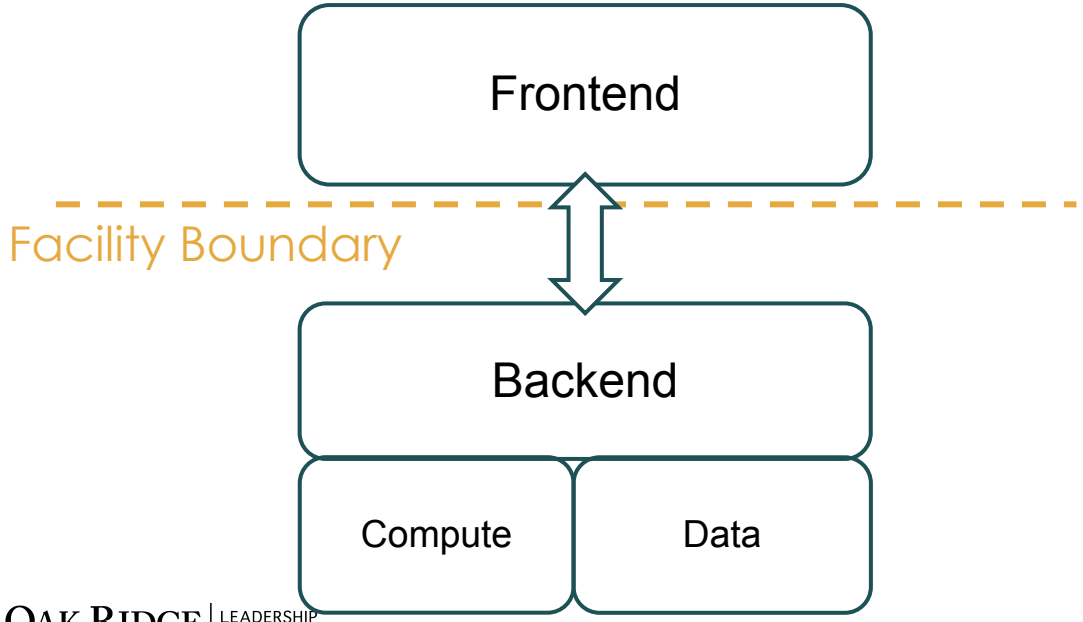
Challenges increase as you go across facilities. This is the IRI solution space.



Arising IRI patterns for data portals

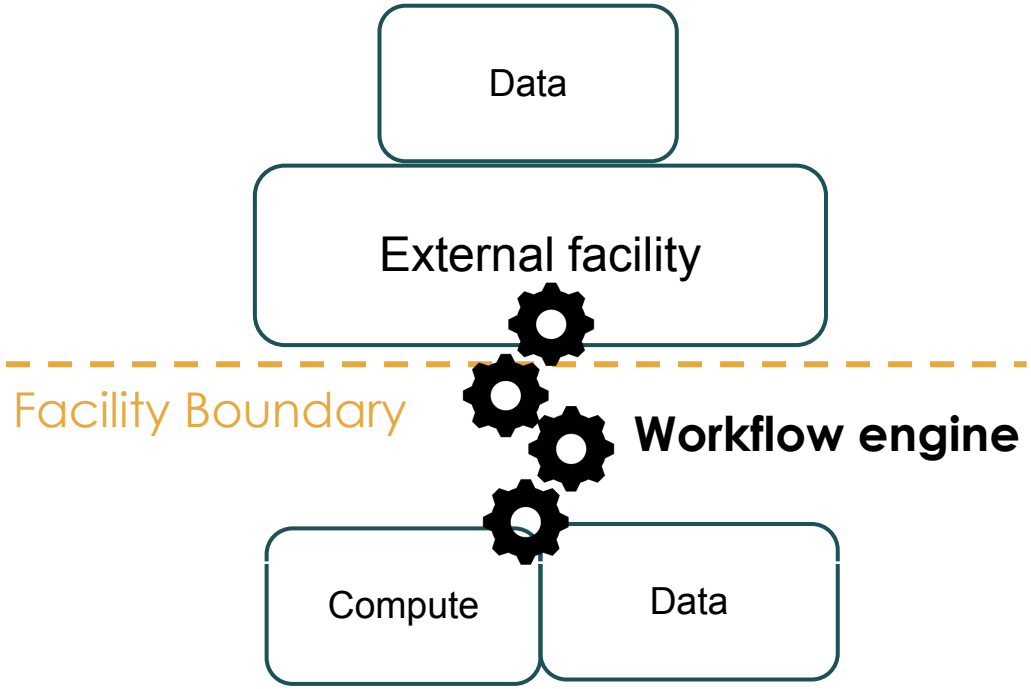
Server-side computing

- Backend provides data and limited compute functions
- Frontend users are limited to specific actions on provided data



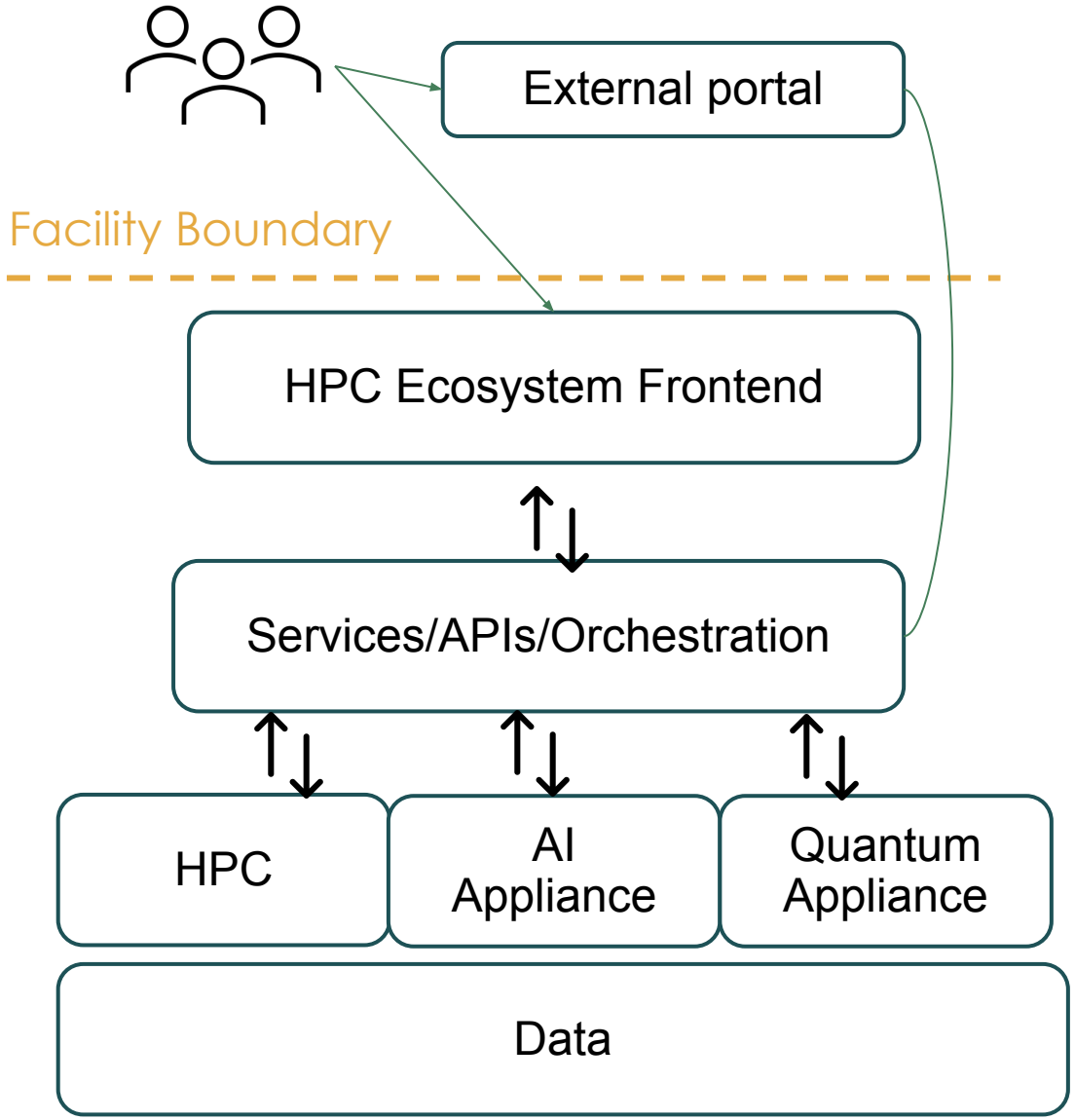
Facility-to-facility

- Data resides at external facility
- Users of external facility utilize a provided workflow engine to move data and access remote compute resources



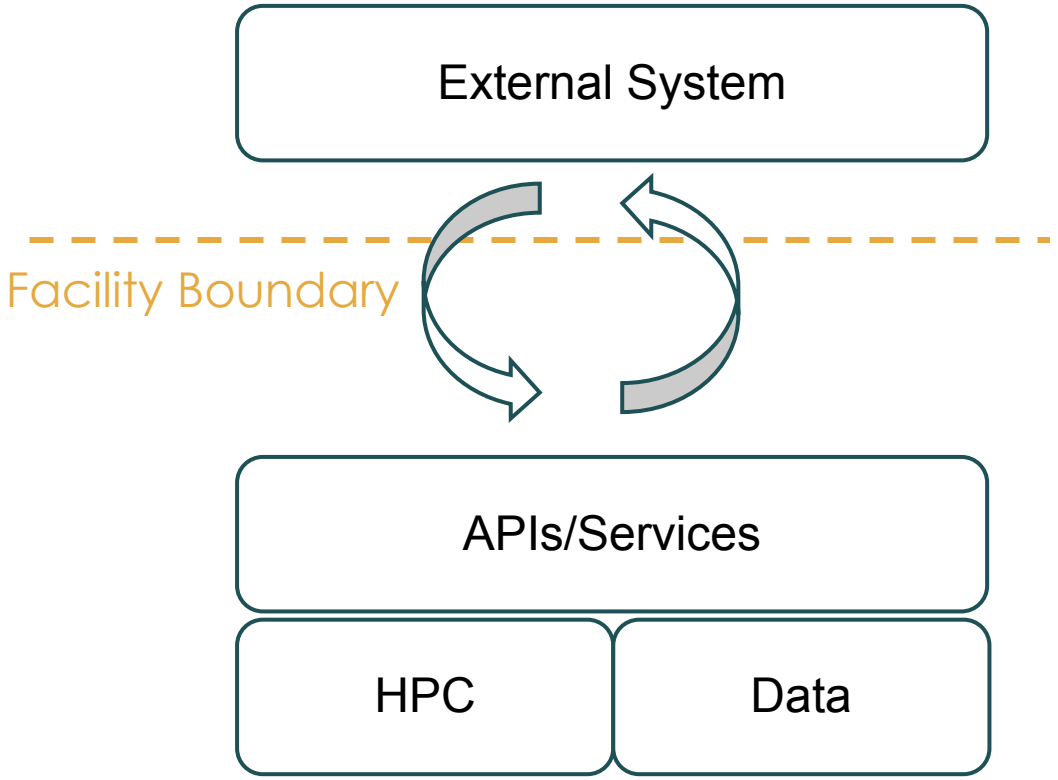
Exploration of a software-driven facility ecosystem

- Decouple systems from services and orchestration layer
- Services and orchestration layer provides access to an array of backend systems
- Decoupling allows services and orchestration to happen "above" target HPC/AI/Quantum systems
- HPC Frontend connects to controlled APIs that drive workflows on the backend systems
- Facility staff can develop and integrate services that plug into the middle layer in support of the diverse user base

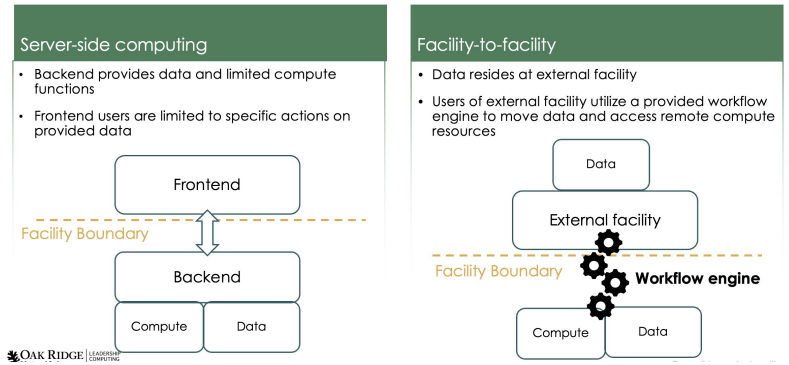


Exploration of services to support external integration

- Operational requirements are still being defined
  - Operational trust between the facility and the external system are needed
- We are exploring a Facility API system and Globus services
  - Interested in how these systems can complement each other
  - Important for ASCR Facilities to provide options
  - AuthN/AuthZ policies for APIs and tokens
- Token management is key to the user experience
  - Can we enable long-lived tokens to external portals with very understood and limited access to facility resources?
  - Globus tokens vs. Facility tokens?
- Identifying certain patterns arising is a key first step:



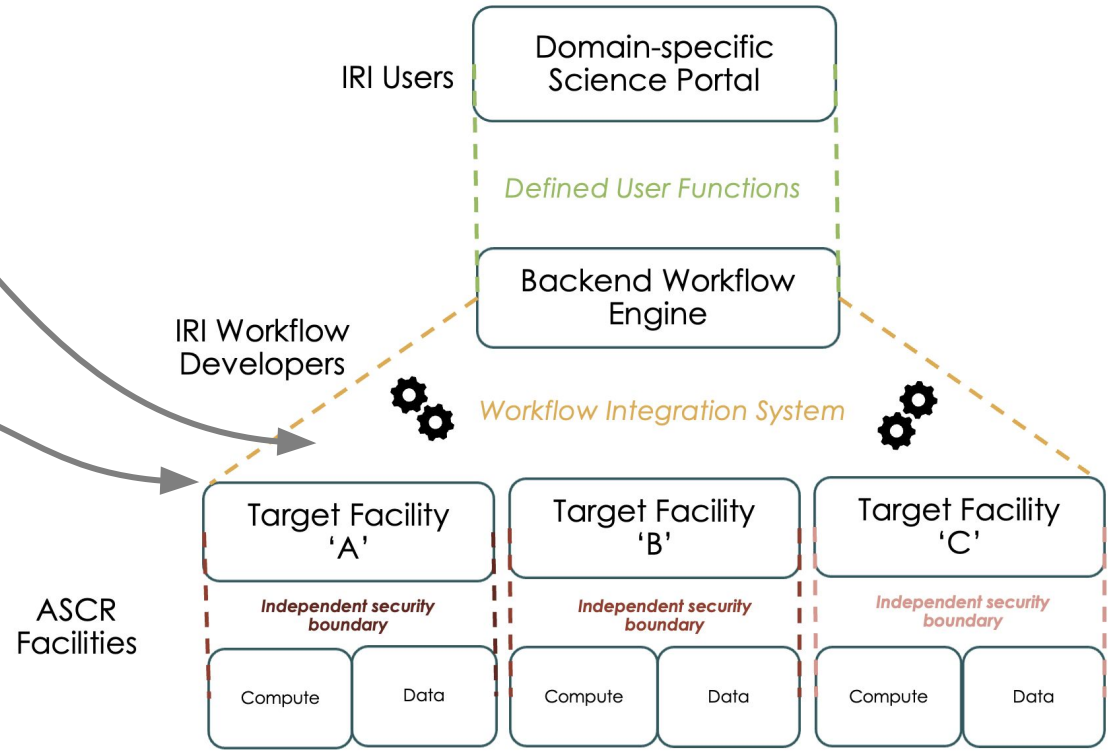
Arising IRI patterns for data portals



OAK RIDGE National Laboratory | LEADERSHIP COMPUTING FACILITY

ResearchOps for IRI

- What do IRI developers need?
  - Policy evolution
  - Technical capabilities
- What should facilities prioritize?
- How do we streamline research across ASCR?
  - People
  - Tools and Infrastructure
- Important to maintain facility uniqueness in terms of capabilities, but also important to drive towards a common IRI user experience



Lightning Talk IV

Globus Platform Interfaces for Automating Science

Kyle Chard
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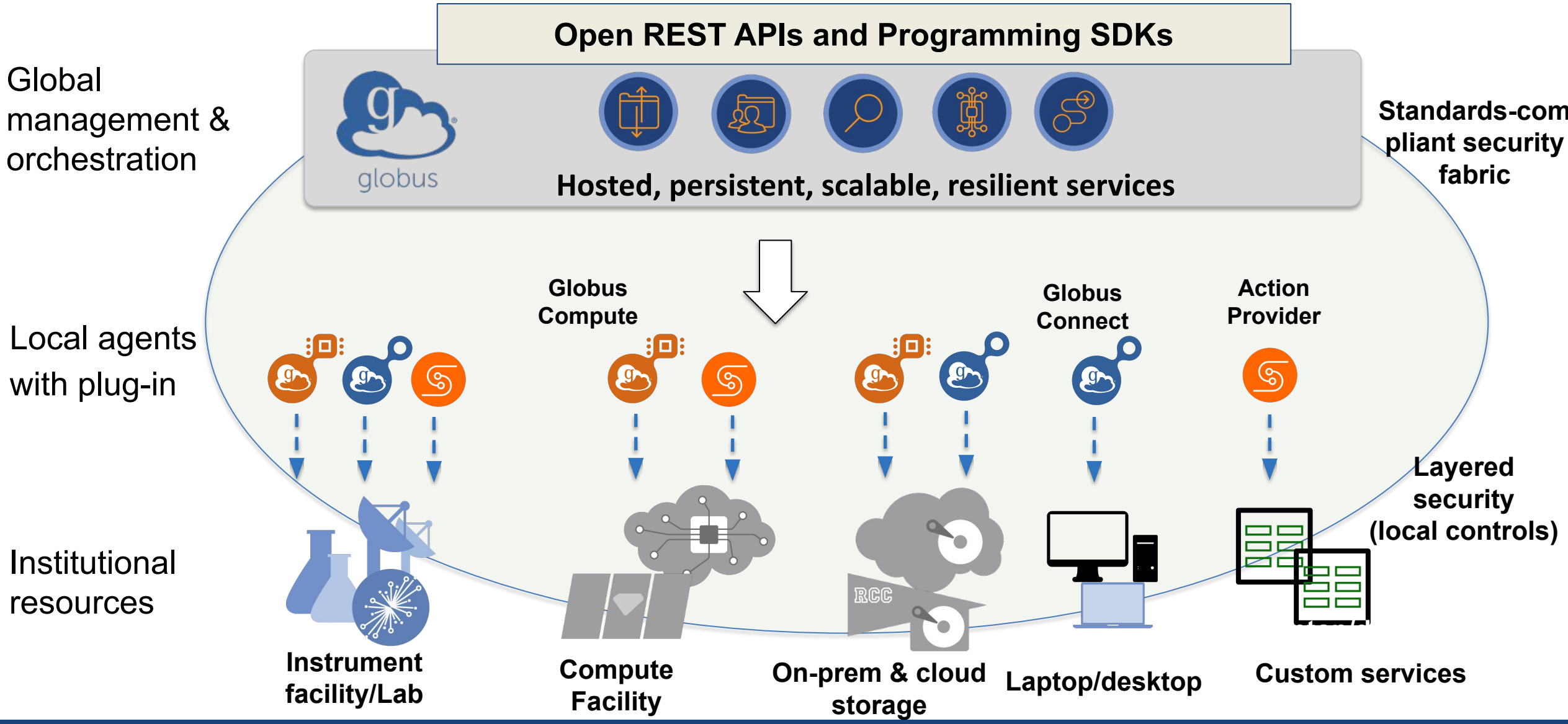
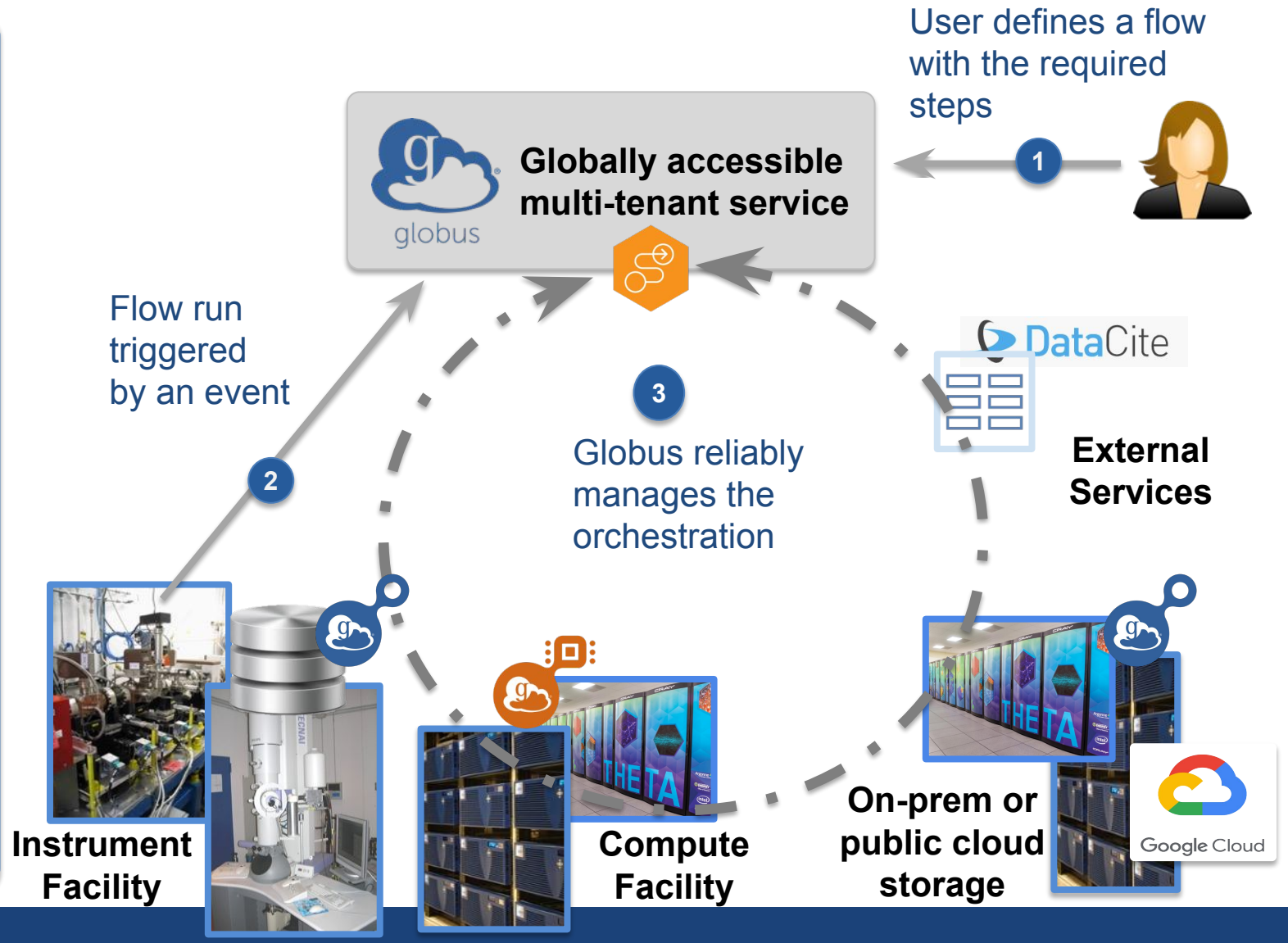
Globus implements a hybrid model for research IT

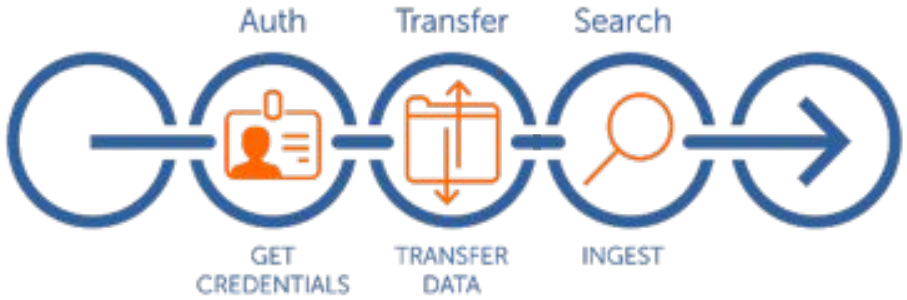


Automating research with Globus Flows

- **Managed reliable task orchestration**
- **Event driven execution model – state machine**
- **Declarative language for flow definition**
- **Extensible for integrating external services via a common asynchronous action API**
  - **/run**
  - **/status**
  - **/cancel**
  - **/release**



APS and ALCF



~20 service accounts with
On-demand access to 56 Polaris nodes

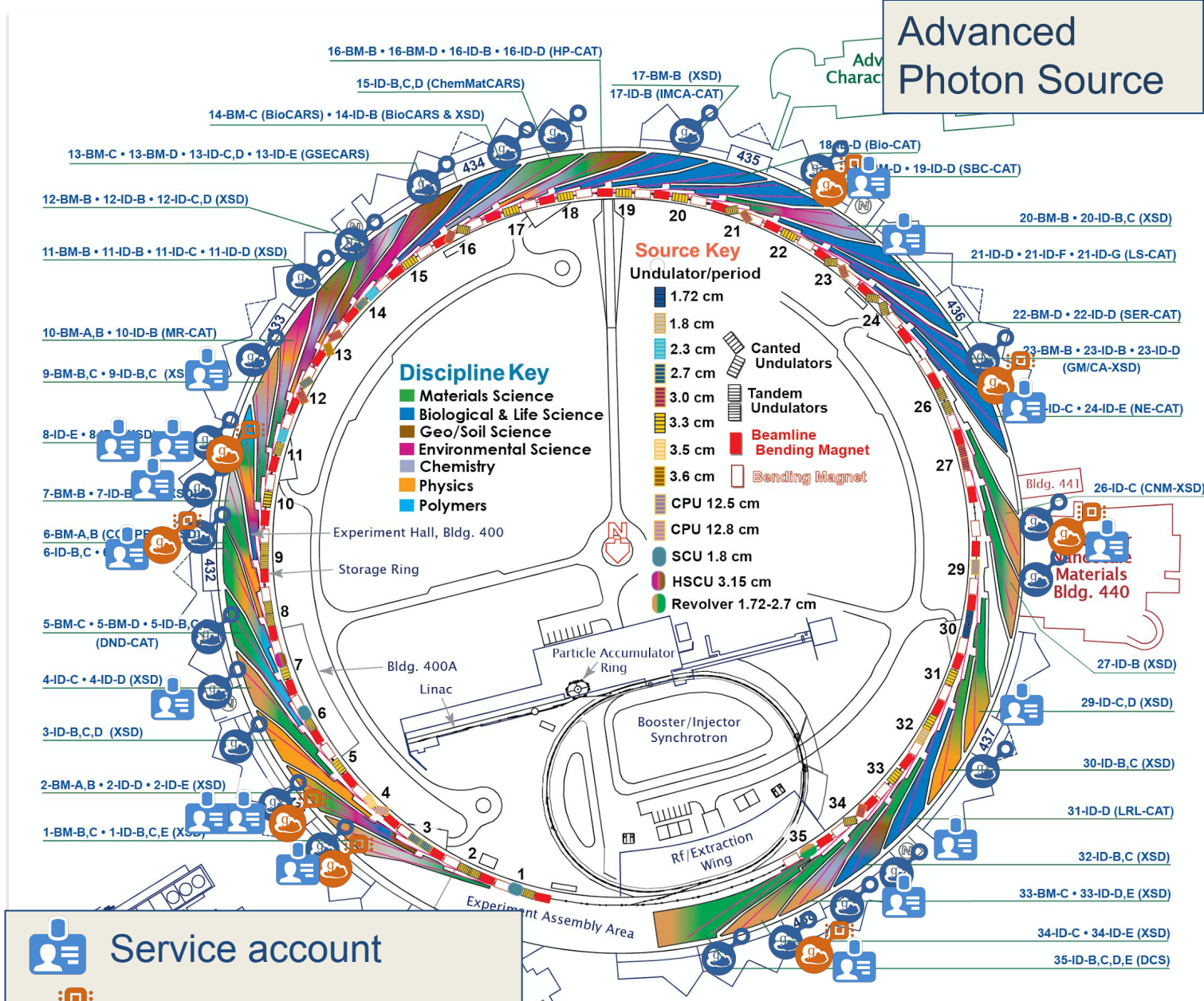
Aurora | Polaris | Eagle store — Argonne Leadership Computing Facility

Bebop Cluster — Laboratory Computing Research Center

Orthros Cluster | APS DM system — APS Computing

Portals

amazon web services

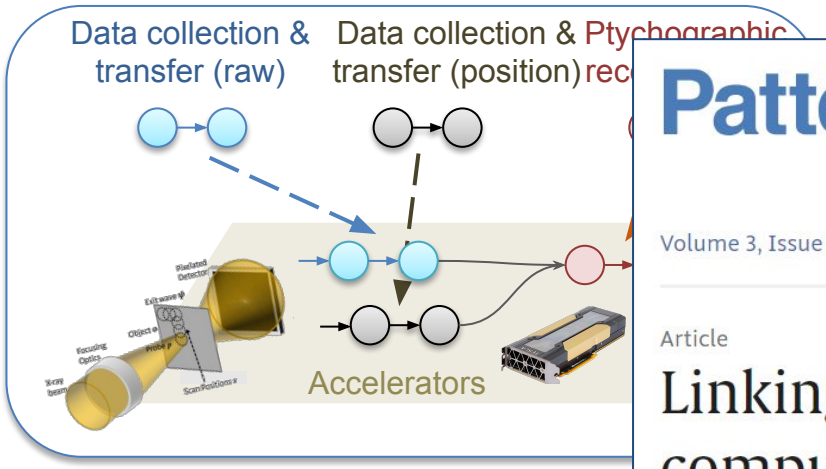


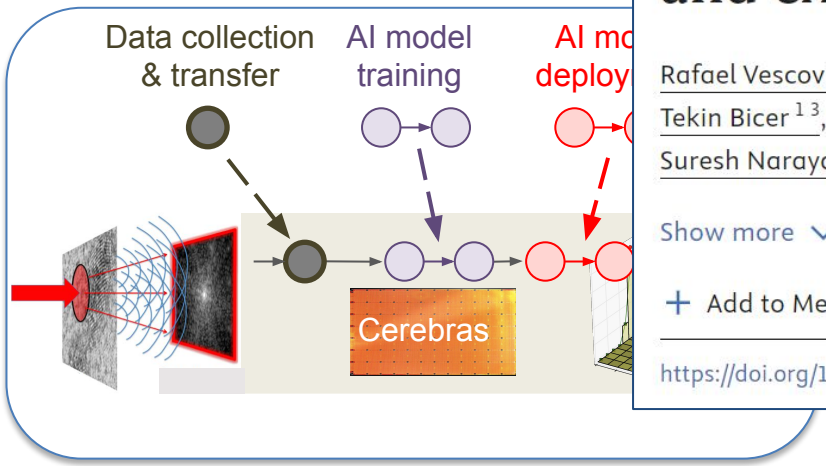
Service account

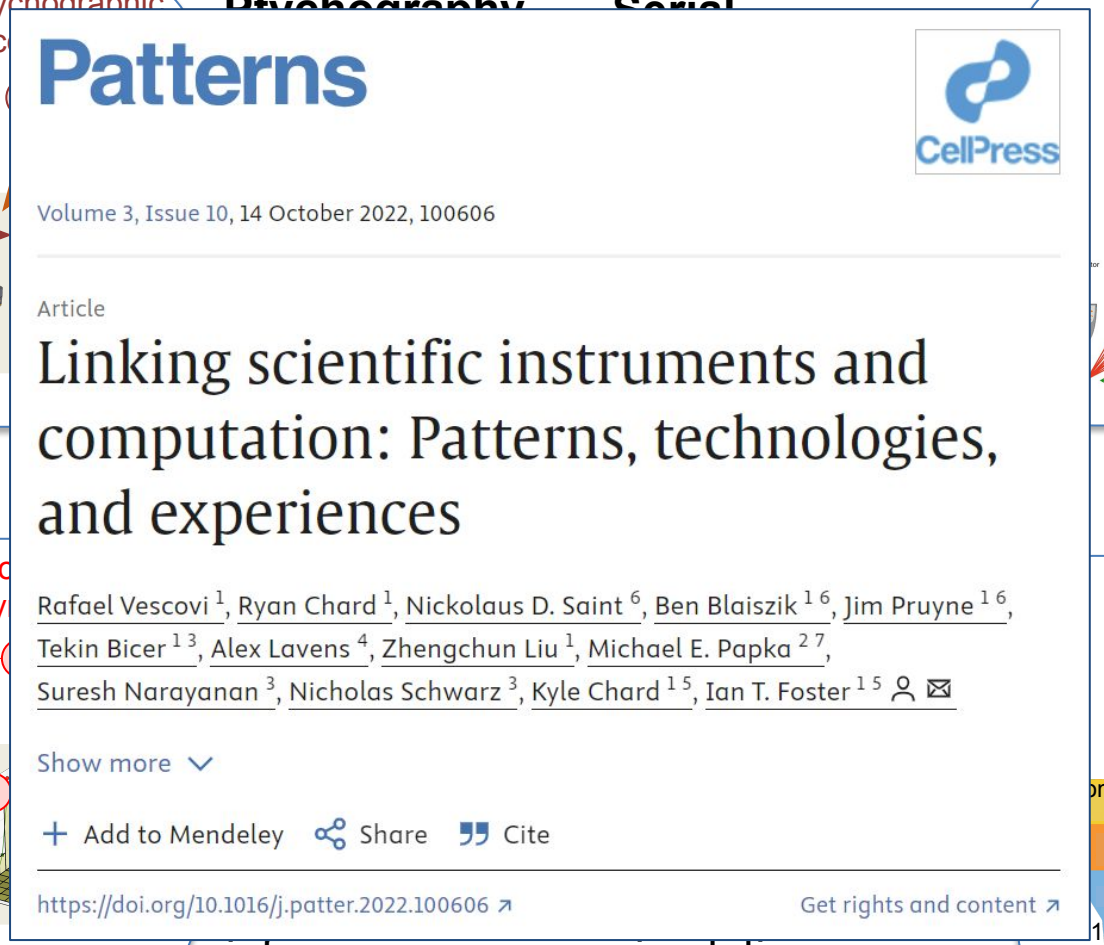
Globus Compute Agent

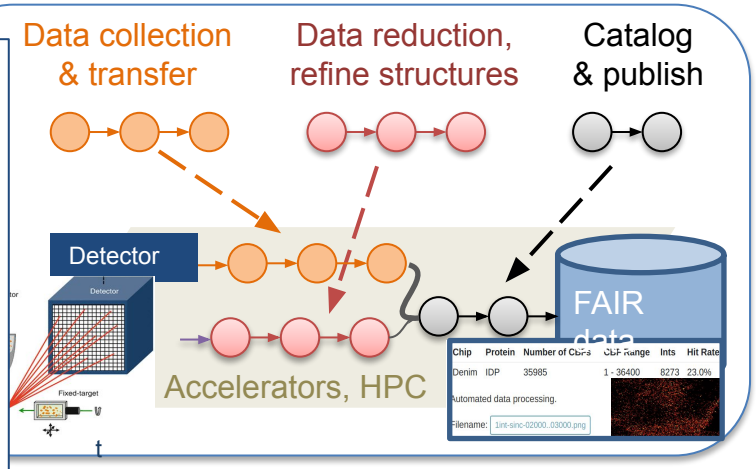
Globus Connect

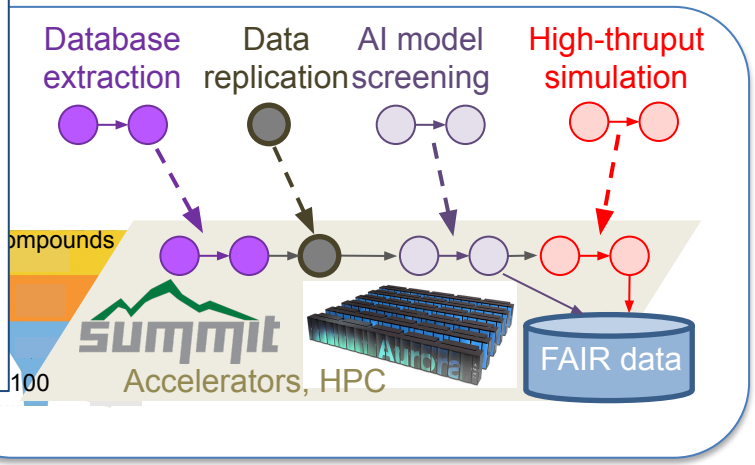
Linking scientific instruments and computation











inference simulation

https://doi.org/10.1016/j.patter.2022.100606

Lightning Talk V

FirecREST: an Open-Source API for HPC

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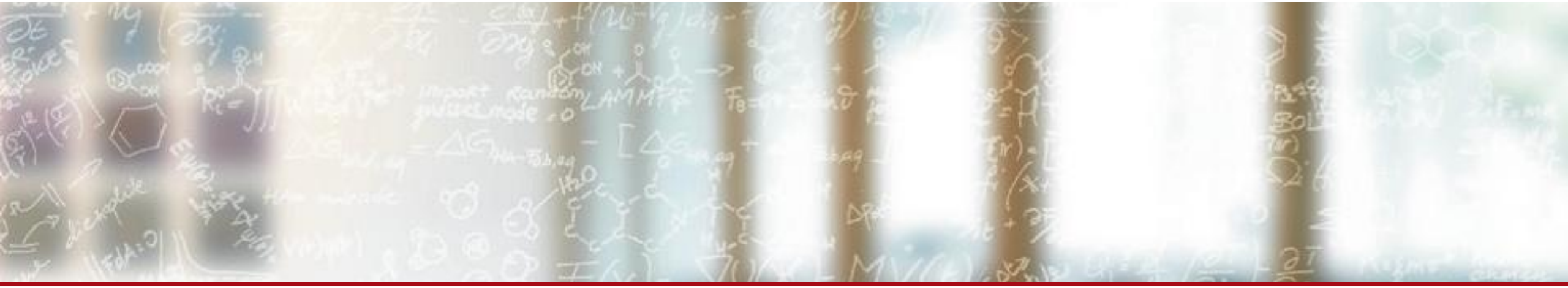
Swiss National Supercomputing Centre

ETH zürich



FirecREST: an open-source API for HPC

Juan Pablo Dorsch (juanpablo.dorsch@cscs.ch)
CSCS - Swiss National Supercomputing Centre
ETH-Zürich

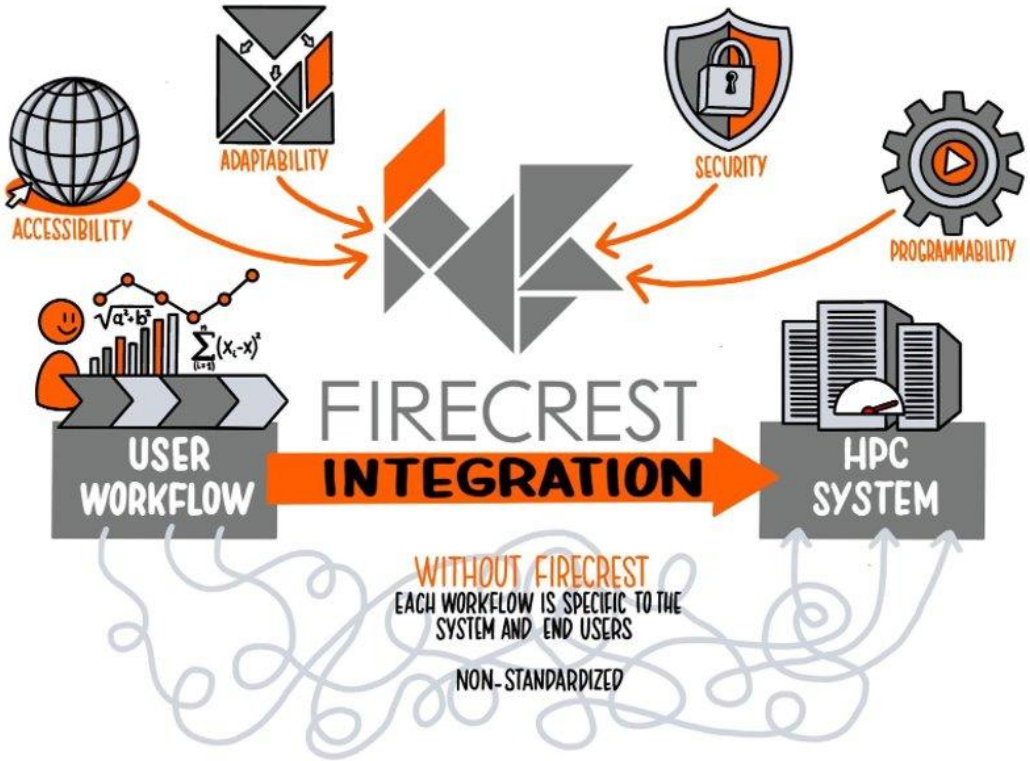
November 21, 2024
SC24
Atlanta, GA, USA

Motivation

- **User community needs**: the HPC user community increasingly requires automated workflows and access to advanced services to streamline their computational tasks
- **Infrastructure Challenges:** Supporting this diverse range of services and workflows poses significant scalability challenges for HPC infrastructure
- **Programming Standards:** These demands highlight the need for standardized programming practices to ensure efficient and consistent usage of HPC resources.

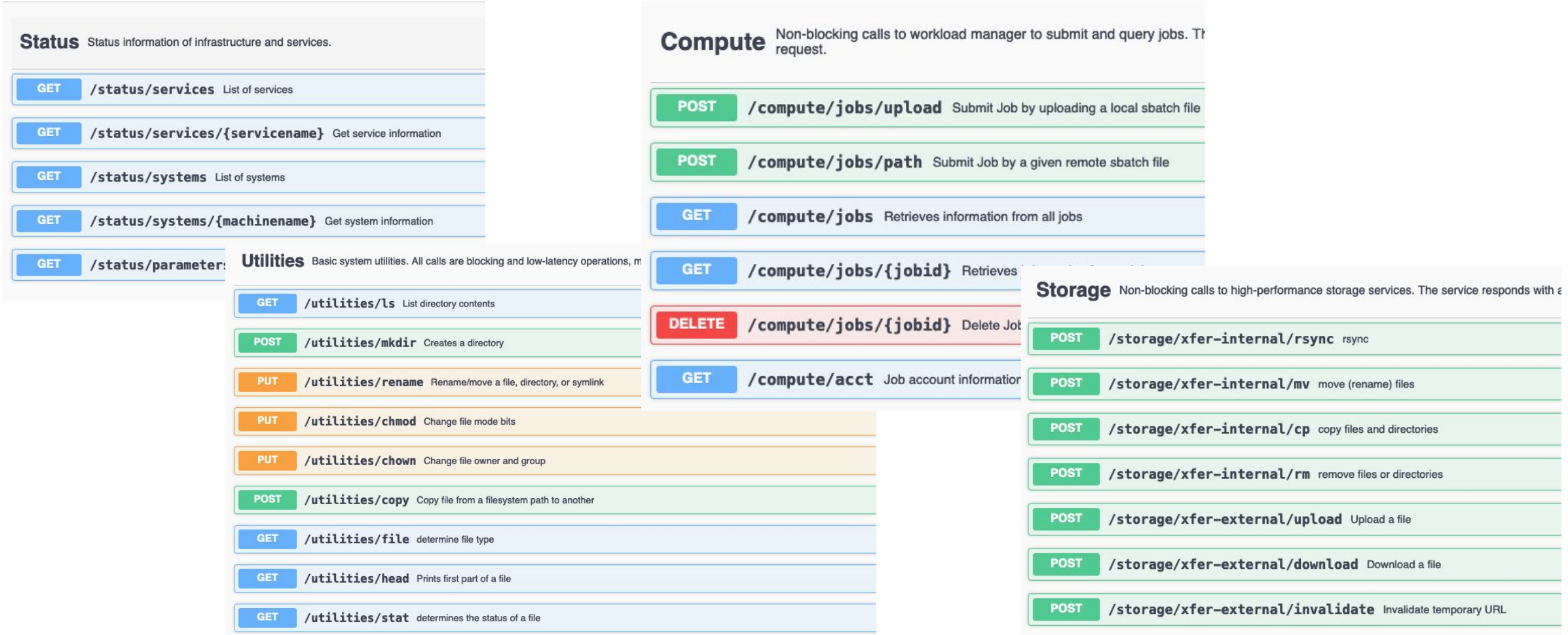
FirecREST features

- **FirecREST is an open-source web-enabled API to HPC resources developed by CSCS**
- Includes abstractions for workload managers and schedulers, data transfer, and common filesystem's operations
- Allows workflow execution and data transfer across supercomputing facilities
- Facilitates workflows support, monitoring and observability



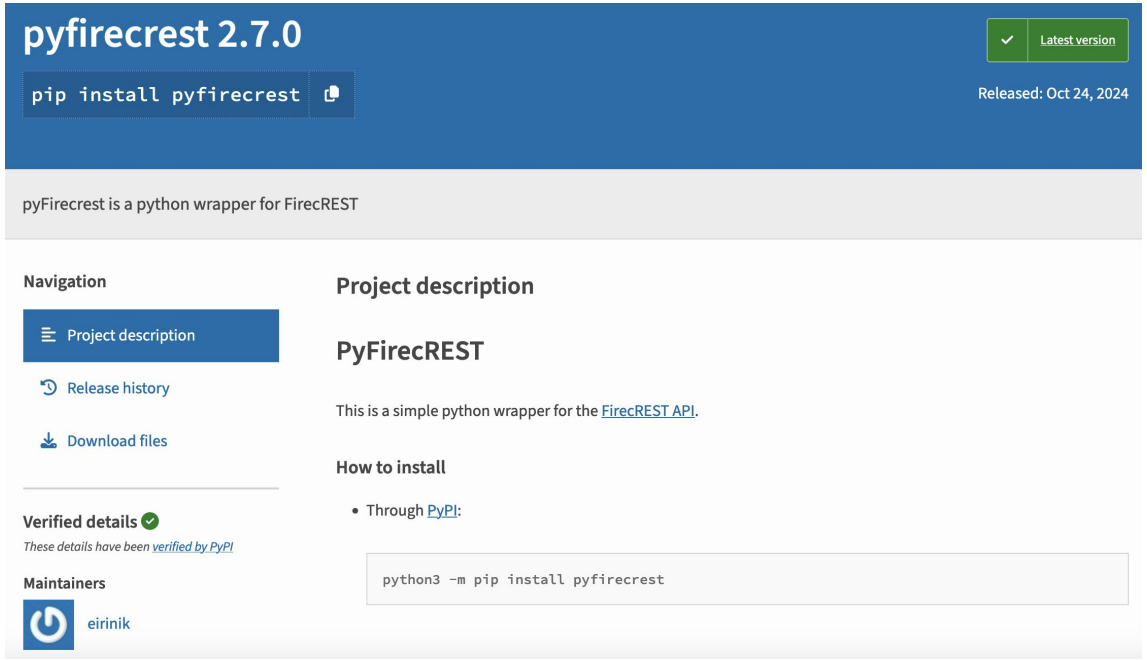
The FirecREST API

- OpenAPI documentation: https://firecrest-api.cscs.ch



pyFirecREST Library

- pyFirecREST is a Python library that wraps FirecREST endpoints for scripting
- Seamless integration with OIDC/OAuth2 for JWT Access Token
- **Facilitates integration with tools that expose APIs or SDKs via Python or scripting languages**



Link to pyFirecREST Docs

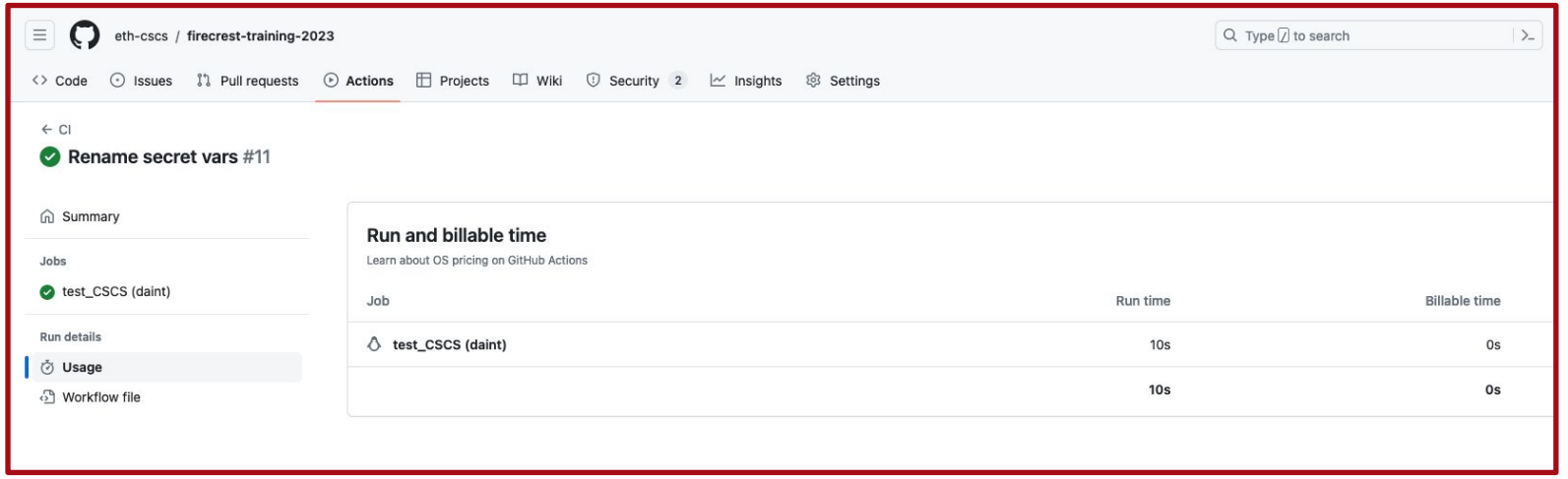
CSCS
Centro Svizzero di Calcolo Scientifico
Swiss National Supercomputing Centre

ETH zürich

FirecREST to streamline services on HPC

FirecREST to streamline services on HPC

- Continuous Integration (CI) Pipelines
  - Running pipelines from the cloud using any CI/CD service
  - Avoids the need for SSH connection to the facility



FirecREST to streamline services on HPC

- Interactive Computing
  - Jupyter Hub's FirecREST Spawner reduces the requirement on the HPC infrastructure side in terms of administration, machine provisioning, networking, etc.
  - Extending the well-known `batchspawner` allows to create JupyterLab Notebooks from the cloud.
  - The “recipe” can be replicated for several HPC systems by changing the configuration to a different system

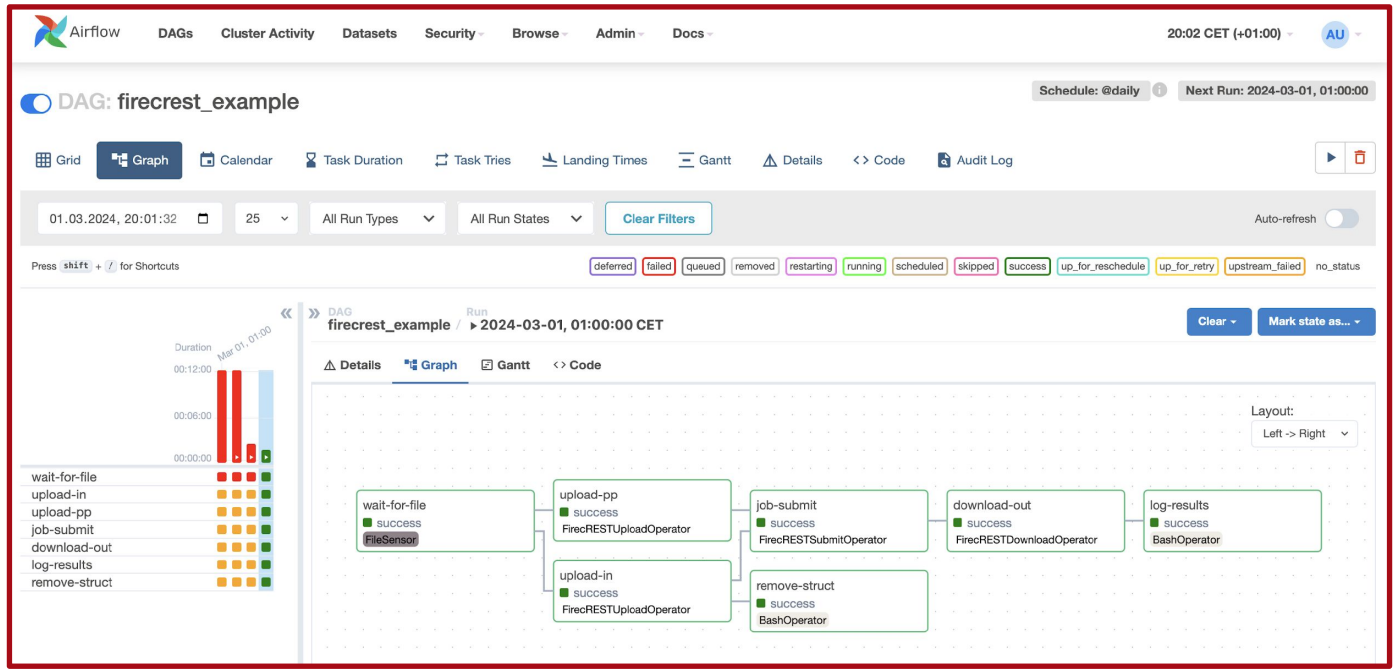
Link to Jupyter's FirecREST Spawner Docs

FirecREST to streamline services on HPC

- Scientific Portals
  - Successful use cases on integrating FirecREST and OpenOnDemand
  - Jupyter Notebooks and Filesystem plugins has been created using FirecREST
  - This way we can decouple OOD from the login node and the infrastructure of the HPC Center

FirecREST to streamline services on HPC

- Workflow Orchestrators
  - Enables an Airflow FirecREST Operator for HPC tasks (submit a job, upload/download data)
  - Create DAGs with those operators and run them from your laptop or the cloud



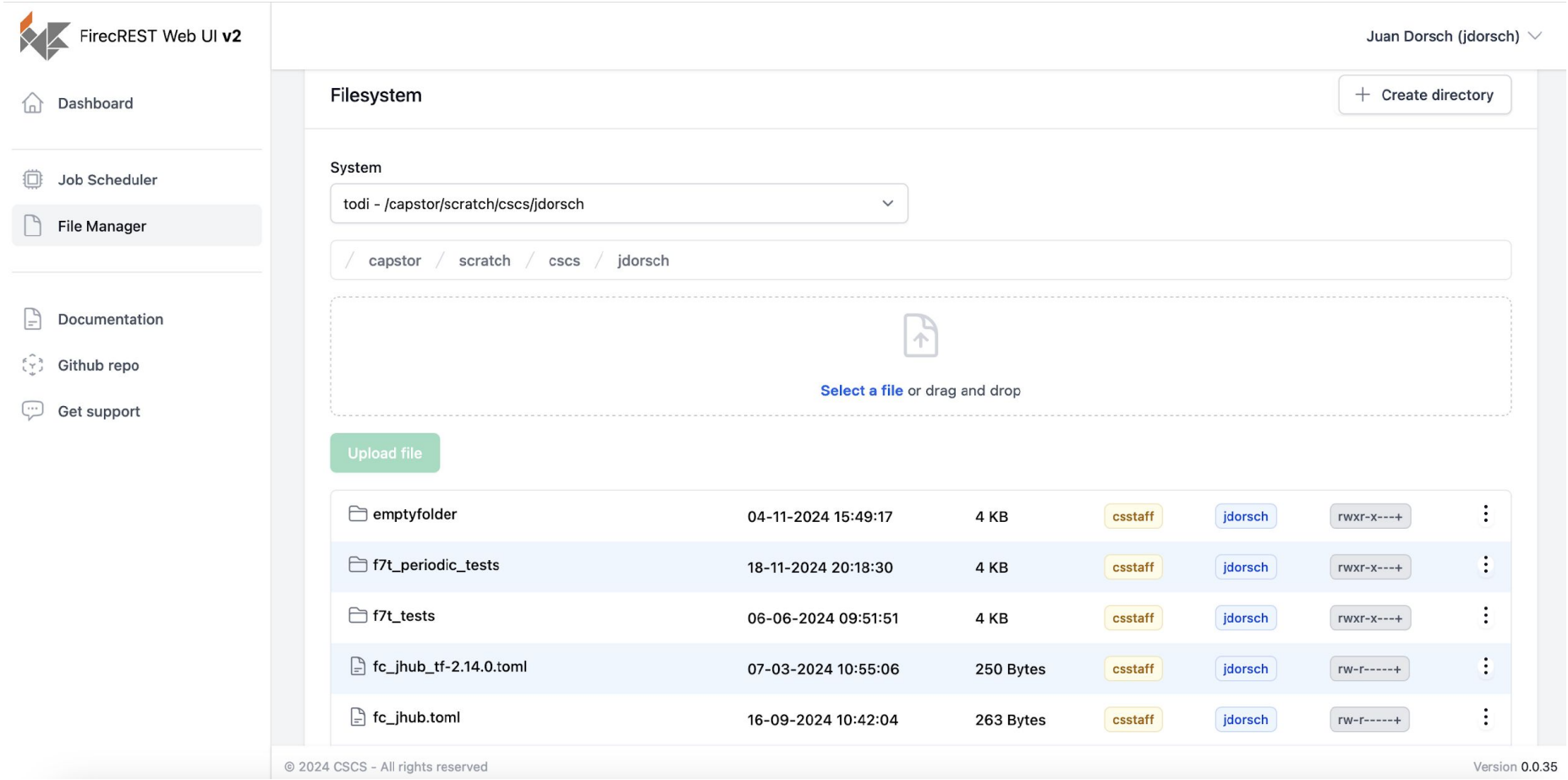
Apache Airflow

nextflow

snakemake

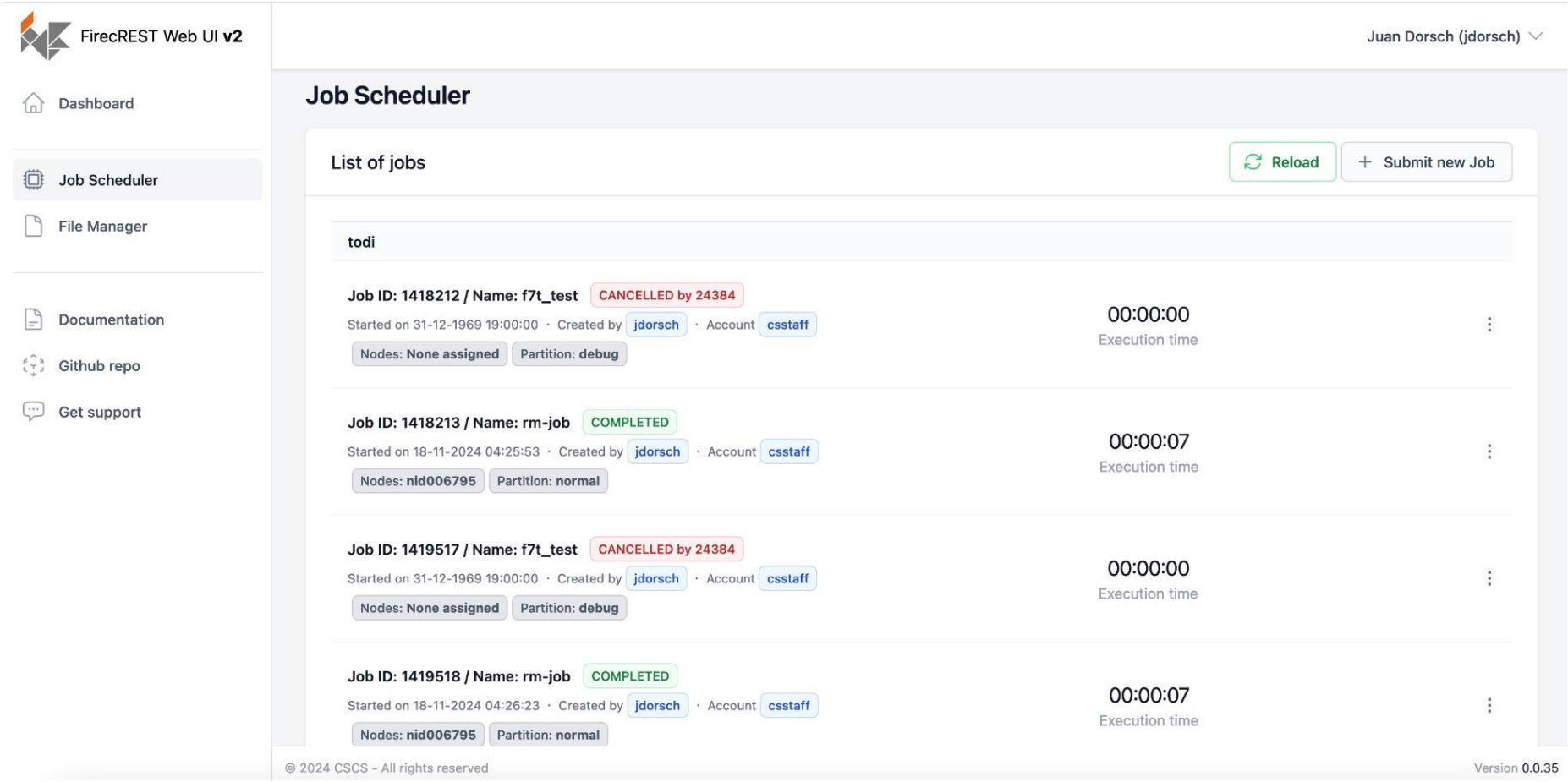
FirecREST to streamline services on HPC

- User Portals



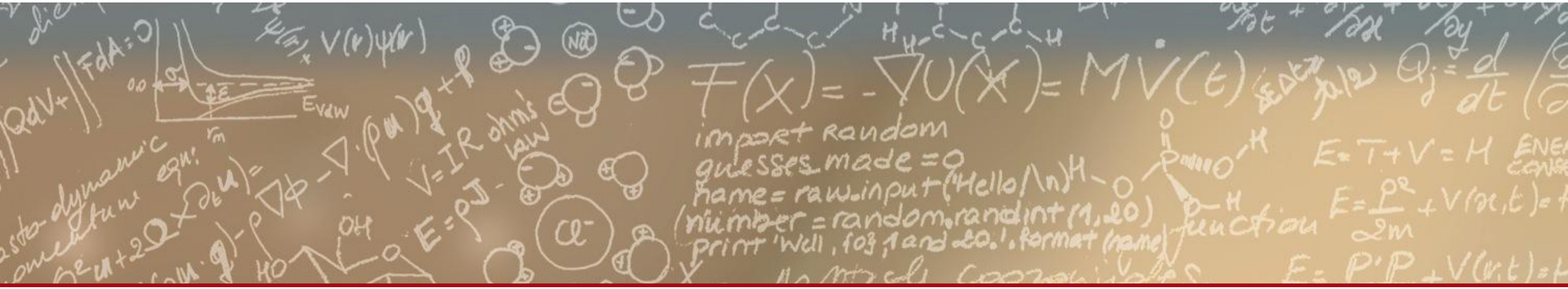
FirecREST to streamline services on HPC

- User Portals



Links and references

- More on FirecREST
  - API Reference: firecrest-api.cscs.ch
  - FirecREST product page at CSCS: products.cscs.ch/firecrest
  - FirecREST public repository: github.com/eth-cscs/firecrest
  - FirecREST Docs (use cases): firecrest.readthedocs.io
  - pyFirecREST and CLI Docs: pyfirecrest.readthedocs.io
  - Join our community on Slack: firecrest-community.slack.com
  - Contact us: firecrest@cscs.ch



Thank you for your attention.

Q&A panel and open discussion

Bjoern Enders
NERSC/LBL

John MacAuley
ESnet

Xi Yang
ESnet

Ryan Prout
OLCF

Juan Pablo Dorsch
CSCS

Kyle Chard
ANL